Multilayer Perceptrons

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Ch. 11 of I2ML (Secs. 11.8 – 11.11 excluded)

Outline

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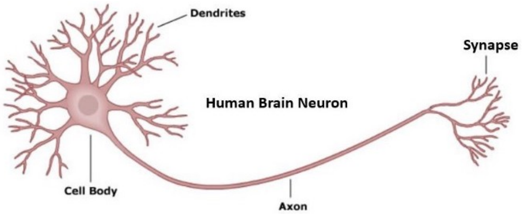
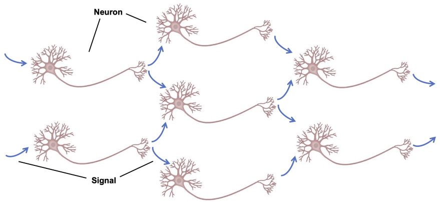
Artificial Neural Networks – I

- Cognitive scientists and neuroscientists: the aim is to understand the functioning of the brain by building models of the natural neural networks in the brain.
- Machine learning researchers: the aim (more pragmatic) is to build better computer systems based on inspirations from studying the brain.
- The human brain is quite different from a computer.
  - a computer generally has one processor
  - the brain is composed of a very large number of processing units, namely, biological neurons (nerve cells)



Artificial Neural Networks – II

- In the brain, neurons are cells within the nervous system that transmit information to other neurons, muscle, or gland cells.
- A human brain has:
  - Large number (10^{11}) of neurons as processing units
  - Large number (10^{4}) of synapses per neuron as memory units
  - Parallel processing capabilities
  - Distributed computation/memory
  - High robustness to noise and failure
- Biological neural networks:

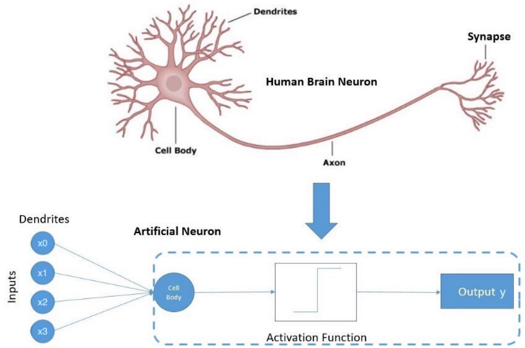


- Artificial neural networks (ANN) mimic some characteristics of the human brain, especially with regard to the computational aspects.

Outline

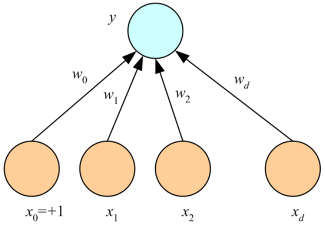
Perceptron – I

- The perceptron (or artificial neuron), a mathematical model of a biological neuron, is the basic processing element in artificial neural networks.



- The single-layer perceptron forms a feedforward neural network, i.e., an ANN where information always moves one direction; it never goes backwards.

Perceptron – II



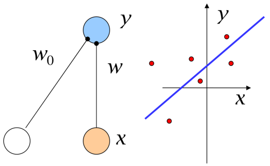
- The output, y, in the simplest case is a weighted sum of the inputs $\mathbf{x} = (x_0, x_1, \ldots, x_d)^T$ (may come from the environment or may be the outputs of other perceptrons):

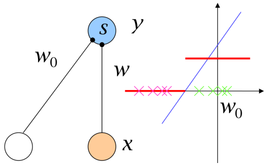
$$y = \sum_{j=1}^{d} w_j x_j + w_0 = \mathbf{w}^T \mathbf{x}$$

  where x_0 is a special bias unit with $x_0 = 1$ and $\mathbf{w} = (w_0, w_1, \ldots, w_d)^T$ is the weight vector with w_0 called the bias weight and w_j, $j = 1, \ldots, d$, called the connection weights or synaptic weights.

What a Perceptron Does

- Regression vs. classification (figures show perceptrons with a univariate input x):





- By using it to implement a linear discriminant function, the perceptron can separate two classes by checking the sign of the output.
  - If we define the threshold (step) function

$$s(a) = \mathbf{1}(a > 0) = \begin{cases} 1 & \text{if } a > 0 \\ 0 & \text{otherwise} \end{cases}$$

we can obtain the following decision rule:

$$\text{Choose } \begin{cases} C_1 & \text{if } s(\mathbf{w}^T\mathbf{x}) = 1 \\ C_2 & \text{otherwise} \end{cases}$$

Sigmoid Function

- Instead of using the threshold function to give a discrete output in $\{0, 1\}$, we may use the sigmoid function

$$\text{sigmoid}(a) = \frac{1}{1 + \exp(-a)}$$

  to give a continuous output in $[0, 1]$:

$$y = \text{sigmoid}(\mathbf{w}^T \mathbf{x})$$

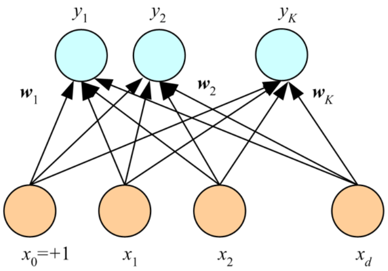
- The output may be interpreted as the posterior probability that the input $\mathbf{x}$ belongs to C_1, which at a later stage can be used, for example, to calculate the risk.

$K > 2$ Outputs - I

- K perceptrons, each with a weight vector $\mathbf{w}_i$:

$$y_i = \sum_{j=1}^{d} w_{ij}x_j + w_{i0} = \mathbf{w}_i^T\mathbf{x} \quad or \quad \mathbf{y} = \mathbf{W}\mathbf{x}$$

  where w_{ij} is the weight from input x_j to output y_i and each row of the $K \times (d+1)$ matrix $\mathbf{W}$ is the weight vector of one perceptron.



- The above function performs a linear transformation from a d-dimensional space (neglecting x_0 since it is constant) to a K-dimensional space.
  - The network can also be used for dimensionality reduction if $K < d$.
- By defining auxiliary inputs, the linear perceptron can also be used for polynomial approximation, i.e., regression, as discussed before.

$K > 2$ Outputs – II

- Classification

$$\text{Choose } C_i \text{ if } y_i = \max_k y_k$$

- If we need the posterior probabilities as well, we can use softmax to define y_i as:

$$y_i = \frac{\exp(\mathbf{w}_i^T \mathbf{x})}{\sum_{k=1}^{K} \exp(\mathbf{w}_k^T \mathbf{x})}$$

Perceptron Learning

- Learning mode:
  - Batch learning: whole sample seen all at once.
  - Online learning: instances seen one by one.
  - Mini-batch learning: between online and batch learning.
- Advantages of online learning:
  - No need to store the whole sample.
  - Can adapt to changes in sample distribution over time.
  - Can adapt to physical changes in system components.
- The error function is not defined over the whole sample $\mathcal{X}$ but on individual instances.
- Starting from randomly initialized weights, the parameters are adjusted a little bit at each iteration to reduce the error without forgetting what was learned previously.
- A complete pass over all the patterns in the training set is called an epoch.

SGD for Regression

- If the error function is differentiable, gradient descent may be applied at each iteration to reduce the error.
- Gradient descent for online learning is also known as stochastic gradient descent (SGD) or online gradient descent.

- For regression, the error on a single instance $(\mathbf{x}^t, r^t)$:

$$E^t(\mathbf{w} \mid \mathbf{x}^t, r^t) = \frac{1}{2}(r^t - y^t)^2 = \frac{1}{2}\left[r^t - (\mathbf{w}^T\mathbf{x}^t)\right]^2$$

  which gives the following online update rule:

$$\Delta w_j^t = -\eta \frac{\partial E^t}{\partial w_j} = -\eta \frac{\partial E^t}{\partial y^t} \frac{\partial y^t}{\partial w_j} = \eta(r^t - y^t)x_j^t$$

  where η is a step size (or learning rate or learning factor) parameter which can be chosen to be decreased gradually over time to facilitate convergence.

SGD for Binary Classification

- For classification, we can use logistic discrimination.
- Logistic for a single instance $(\mathbf{x}^t, r^t)$, where $r^t = 1$ if $\mathbf{x}^t \in C_1$ and $r^t = 0$ if $\mathbf{x}^t \in C_2$, gives the output:
$$y^t = \text{sigmoid}(\mathbf{w}^T \mathbf{x}^t)$$
- Likelihood:
$$L = (y^t)^{r^t} (1 - y^t)^{1-r^t}$$
- Cross-entropy error function:
$$E^t(\mathbf{w} \mid \mathbf{x}^t, r^t) = -\log L = -r^t \log y^t - (1 - r^t) \log(1 - y^t)$$
- Online update rule:
$$\Delta w_j^t = -\eta \frac{\partial E^t}{\partial w_j} = \eta (r^t - y^t) x_j^t$$
which is the same as the equations we saw in last lecture except that we do not sum over all of the instances but update after a single instance.

SGD for Multi-Class Classification

- Softmax for a single instance $(\mathbf{x}^t, \boldsymbol{r}^t)$, where $r_i^t = 1$ if $\mathbf{x}^t \in C_i$ and 0 otherwise, gives the outputs:
$$y_i^t = \frac{\exp(\mathbf{w}_i^T \mathbf{x}^t)}{\sum_{k=1}^K \exp(\mathbf{w}_k^T \mathbf{x}^t)}$$
- Likelihood:
$$L = \prod_i (y_i^t)^{r_i^t}$$
- Cross-entropy error function:
$$E^t(\{\mathbf{w}_i\} \mid \mathbf{x}^t, \mathbf{r}^t) = -\log L = -\sum_i r_i^t \log y_i^t$$
- Online update rule:
$$\Delta w_{ij}^t = \eta(r_i^t - y_i^t)x_j^t$$
- All the update equations have the same form
$$\text{Update} = \text{LearningRate} \times \underbrace{(\text{DesiredOutput} - \text{ActualOutput})}_{\text{the error term for output unit } i} \times \text{Input}$$

Perceptron Learning Algorithm

```
For $i = 1, \ldots, K$
    For $j = 0, \ldots, d$
        $w_{ij} \leftarrow$ rand$(-0.01, 0.01)$
Repeat
    For all $(\boldsymbol{x}^t, r^t) \in \mathcal{X}$ in random order
        For $i = 1, \ldots, K$
            $o_i \leftarrow 0$
            For $j = 0, \ldots, d$
                $o_i \leftarrow o_i + w_{ij} x_j^t$
        For $i = 1, \ldots, K$
            $y_i \leftarrow \exp(o_i) / \sum_k \exp(o_k)$
        For $i = 1, \ldots, K$
            For $j = 0, \ldots, d$
                $w_{ij} \leftarrow w_{ij} + \eta (r_i^t - y_i) x_j^t$
Until convergence
```

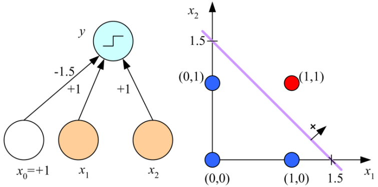
Outline

Learning Boolean Function AND

- In a Boolean function, the inputs are binary and the output is 1 if the corresponding function value is true and 0 otherwise.
- Learning a Boolean function is a two-class classification problem.
- AND function with 2 inputs and 1 output:

x_1	x_2	r
0	0	0
0	1	0
1	0	0
1	1	1

- Perceptron for AND and its geometric interpretation:



Learning Boolean Function XOR – I

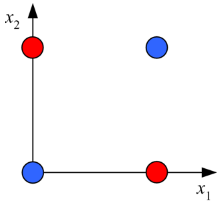
- A simple perceptron can only learn linearly separable Boolean functions such as AND and OR but not linearly nonseparable functions such as XOR.
- XOR function with 2 inputs and 1 output:

x_1	x_2	r
0	0	0
0	1	1
1	0	1
1	1	0

Learning Boolean Function XOR – II

- There do not exist w_0, w_1, w_2 that satisfy the following inequalities:

$$\begin{aligned} w_0 &\leq 0 \\ w_2 + w_0 &> 0 \\ w_1 + w_0 &> 0 \\ w_1 + w_2 + w_0 &\leq 0 \end{aligned}$$



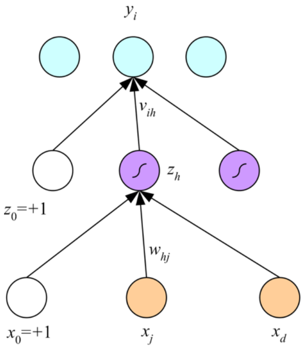
- This result is not surprising since the VC dimension of a line (in two dimensions) is three. With two binary inputs there are four cases, and thus there exist problems with two inputs that are not solvable using a line; XOR is one of them.

Outline

Multilayer Perceptrons

- A single-layer perceptron can only approximate linear functions of the input and cannot solve problems like XOR, where the discrimininant is nonlinear. Similarly, a perceptron cannot be used for nonlinear regression.

- A multilayer perceptron (MLP) (a.k.a. deep feedforward neural networks) has a hidden layer between the input and output layers.
- MLP can implement nonlinear discriminants (for classification) and nonlinear regression functions (for regression).
- We call this a two-layer network because the input layer performs no computation.



Forward Propagation – I

- Input-to-hidden:

$$z_h = \text{sigmoid}(\mathbf{w}_h^T \mathbf{x}) = \frac{1}{1 + \exp\left[-(\sum_{j=1}^{d} w_{hj} x_j + w_{h0})\right]}$$

  - The hidden units must implement a nonlinear function called activation function (e.g., sigmoid or hyperbolic tangent $\tanh(\cdot)$ (ranges from -1 to $+1$, instead of 0 to $+1$)) or else it is equivalent to a simple perceptron (linear combination of linear combinations is another linear combination). The activation function is an abstraction representing the rate of action potential firing in the nueron cell.
  - Sigmoid can be seen as a continuous, differentiable version of thresholding.

- Hidden-to-output:

$$y_i = \mathbf{v}_i^T \mathbf{z} = \sum_{h=1}^{H} v_{ih} z_h + v_{i0}$$

  - Regression: linear output units.
  - Classification: a sigmoid unit (for $K = 2$) or K output units with softmax (for $K > 2$).

Forward Propagation – II

- The hidden units make a nonlinear transformation from the d-dimensional input space to the H-dimensional space spanned by the hidden units.
- In the new H-dimensional space, the output layer implements a linear function.
- Multiple hidden layers may be used for implementing more complex functions of the inputs, but learning the network weights in such deep networks will be more complicated (to be considered later in the topic of Deep Learning Models).

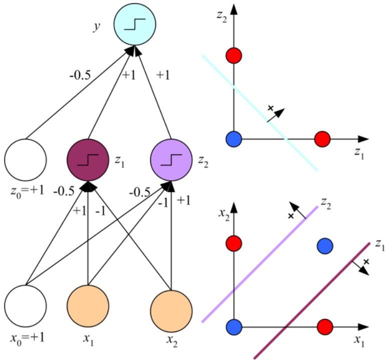
- MLP's are sometimes colloquially referred to as "vanilla" neural networks, especially when they have a single hidden layer.

MLP for XOR

- Any Boolean function can be represented as a disjunction of conjunctions, e.g.

  $$x_1 \text{ XOR } x_2 = (x_1 \text{ AND } \neg x_2) \text{ OR } (\neg x_1 \text{ AND } x_2)$$

  which can be implemented by an MLP with one hidden layer.
- Two perceptrons can in parallel implement the two AND, and another perceptron on top can OR them together.
- The hidden units and the output have the threshold activation function $s(\cdot)$ with threshold at 0.



MLP as a Universal Approximator

- The result for arbitrary Boolean functions can be extended to the continuous case.
- Universal approximation theorem:
  An MLP with one hidden layer can approximate any continuous function on any compact subset of $\mathbf{R}^n$, under mild assumptions on the activation function, given sufficiently many hidden units.

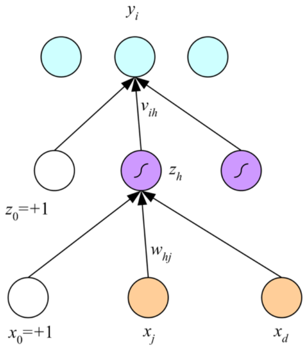
Backpropagation Learning Algorithm

- Training a MLP is the same as training a simple perceptron; the only difference is that now the output is a nonlinear function of the input due to the nonlinear activation function in the hidden units.
- Extension of the perceptron learning algorithm to multiple layers by error backpropagation (backward propagation) from the outputs back to the inputs.
- Learning of hidden-to-output weights:
  Like simple perceptron learning by treating the hidden units as inputs

$$\frac{\partial E}{\partial v_{ih}} = \frac{\partial E}{\partial y_i}\frac{\partial y_i}{\partial v_{ih}}$$

- Learning of input-to-hidden weights:
  Applying the chain rule to calculate the gradient

$$\frac{\partial E}{\partial w_{ij}} = \frac{\partial E}{\partial y_i}\frac{\partial y_i}{\partial z_h}\frac{\partial z_h}{\partial w_{hj}}$$



MLP Learning for Nonlinear Regression With Single Output – I

- Assuming a single output:

$$y^t = \sum_{h=1}^{H} v_h z_h^t + v_0$$

  where $z_h^t = \text{sigmoid}(\mathbf{w}_h^T \mathbf{x}^t)$.

- Error function over entire training sample:

$$E(\mathbf{W}, \mathbf{v} \mid \mathcal{X}) = \frac{1}{2} \sum_t (r^t - y^t)^2$$

- Update rule for second-layer weights:

$$\Delta v_h = -\eta \sum_t \frac{\partial E^t}{\partial y^t} \frac{\partial y^t}{\partial v_h} = \eta \sum_t (r^t - y^t) z_h^t$$

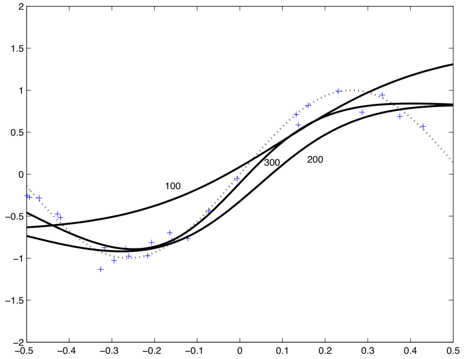
MLP Learning for Nonlinear Regression With Single Output – II

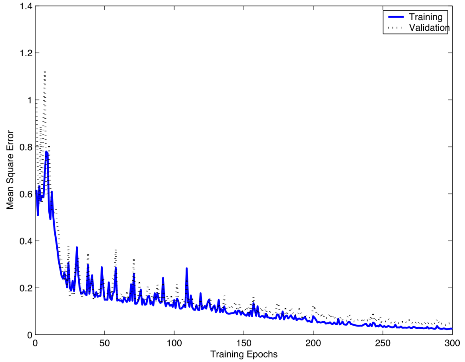
- Update rule for first-layer weights:

$$
\begin{aligned}
\Delta w_{hj} &= -\eta \frac{\partial E}{\partial w_{hj}} \\
&= -\eta \sum_t \frac{\partial E^t}{\partial y^t} \frac{\partial y^t}{\partial z_h^t} \frac{\partial z_h^t}{\partial w_{hj}} \\
&= -\eta \sum_t -(r^t - y^t) \times v_h \times z_h^t(1 - z_h^t) x_j^t \\
&= \eta \sum_t (r^t - y^t) v_h z_h^t (1 - z_h^t) x_j^t
\end{aligned}
$$

- The $(r^t - y^t)v_h$ acts like the error term for hidden unit h. $(r^t - y^t)$ is the error in the output which is backpropagated from the output to the hidden unit weighted by the "responsibility" of the hidden unit as given by its weight v_h.
- Either (mini-)batch learning or online learning may be carried out.

Example





Evolution of regression function and error over epochs

MLP Learning for Nonlinear Regression With Multiple Outputs – I

- When there are multiple output units, a number of regression problems are learned at the same time.
- Outputs:

$$y_i^t = \sum_{h=1}^{H} v_{ih} z_h^t + v_{i0}$$

- Error function:

$$E(\mathbf{W}, \mathbf{V} \mid \mathcal{X}) = \frac{1}{2} \sum_t \sum_i (r_i^t - y_i^t)^2$$

MLP Learning for Nonlinear Regression With Multiple Outputs – II

- Update rule for second-layer weights:

$$\Delta v_{ih} = \eta \sum_t (r_i^t - y_i^t) z_h^t$$

- Update rule for first-layer weights:

$$\Delta w_{hj} = \eta \sum_t \left[\sum_i (r_i^t - y_i^t) v_{ih} \right] z_h^t (1 - z_h^t) x_j^t$$

The $\sum_i (r_i^t - y_i^t) v_{ih}$ is the accumulated backpropagated error of hidden unit h from all output units.

Algorithm

```
Initialize all $v_{ih}$ and $w_{hj}$ to rand$(-0.01, 0.01)$
Repeat
    For all $(\boldsymbol{x}^t, r^t) \in \mathcal{X}$ in random order
        For $h = 1, \ldots, H$
            $z_h \leftarrow \mathrm{sigmoid}(\boldsymbol{w}_h^T \boldsymbol{x}^t)$
        For $i = 1, \ldots, K$
            $y_i = \boldsymbol{v}_i^T \boldsymbol{z}$
        For $i = 1, \ldots, K$
            $\Delta \boldsymbol{v}_i = \eta(r_i^t - y_i^t)\boldsymbol{z}$
        For $h = 1, \ldots, H$
            $\Delta \boldsymbol{w}_h = \eta(\sum_i (r_i^t - y_i^t) v_{ih}) z_h (1 - z_h) \boldsymbol{x}^t$
        For $i = 1, \ldots, K$
            $\boldsymbol{v}_i \leftarrow \boldsymbol{v}_i + \Delta \boldsymbol{v}_i$
        For $h = 1, \ldots, H$
            $\boldsymbol{w}_h \leftarrow \boldsymbol{w}_h + \Delta \boldsymbol{w}_h$
Until convergence
```

The weights are initialized to small random values, e.g., in the range $[-0.01, 0.01]$, so as not to saturate the sigmoids.

MLP Learning for Nonlinear Two-Class Discrimination

- Output:

$$y^t = \text{sigmoid}\Big(\sum_{h=1}^{H} v_h z_h^t + v_0\Big)$$

  which approximate the posterior probabilities $P(C_1 \mid \mathbf{x}^t)$
- Error function:

$$E(\mathbf{W}, \mathbf{v} \mid \mathcal{X}) = -\sum_t \Big[r^t \log y^t + (1 - r^t) \log(1 - y^t) \Big]$$

- Update rules:

$$\Delta v_h = \eta \sum_t (r^t - y^t) z_h^t$$

$$\Delta w_{hj} = \eta \sum_t (r^t - y^t) v_h z_h^t (1 - z_h^t) x_j^t$$

- As in the simple perceptron, the update equations for regression and classification are identical.

MLP Learning for Nonlinear Multi-Class Discrimination

- Outputs:

$$y_i^t = \frac{\exp(o_i^t)}{\sum_i \exp(o_k^t)}$$

which approximate the posterior probabilities $P(C_i \mid \mathbf{x}^t)$, where $o_i^t = \sum_{h=1}^{H} v_{ih} z_h^t + v_{i0}$

- Error function:

$$E(\mathbf{W}, \mathbf{V} \mid \mathcal{X}) = -\sum_t \sum_i r_i^t \log y_i^t$$

- Update rules:

$$\Delta v_{ih} = \eta \sum_t (r_i^t - y_i^t) z_h^t$$

$$\Delta w_{hj} = \eta \sum_t \left[\sum_i (r_i^t - y_i^t) v_{ih} \right] z_h^t (1 - z_h^t) x_j^t$$

MLP With Multiple Hidden Layers

- It is possible to have multiple hidden layers each with its own weights and applying the sigmoid function to its weighted sum.
- It constitutes a feedforward neural network.
- Training such a network can be implemented in a similar way.