

6 Neural Networks

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Abstract

This chapter introduces how we can dealing with non-linear hypotheses with neural network. Although because I have completed the dedicated course “Neural networks for machine learning” on Coursera, please see this course for more explicit details (to avoid duplication). This chapter predominately discusses neural networks for classification.

6.1 Key Remarks

1. Neural networks are one of a few ML algorithms where we continue to improve our prediction accuracy as we increase the number of training examples (most others tend to level off even if we increase the data by a significant amount).
2. Build models that use hardware as efficiently as possible (that way when hardware improves your learning speeds up essentially for free).
3. Set a baseline as the fastest your code can ever run, i.e. the speed of light, or in speech recognition it's 0% WER (improving speed by 10x on already badly written code is not an effective way to analyse this).
4. As discussed at <https://youtu.be/MVyauNNinC0?t=36m18s>, one of the best ways to train a DNN is to try to fool/trick them.

6.2 Representation

Notation 1. **Activation units and vector representation of neural networks**

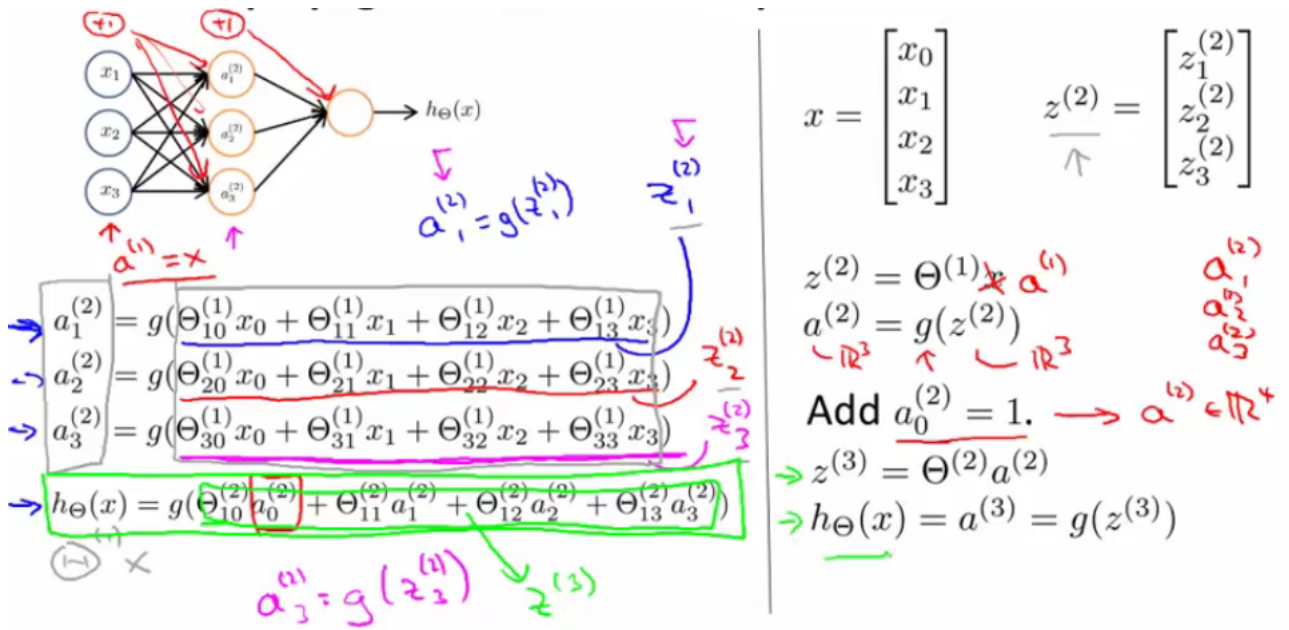


Figure 6.1: A network with s_j units in layer j , s_{j+1} units in layer $j + 1$, then $\Theta^{(j)}$ will be of dimension $s_{j+1} \times (s_j + 1)$. The process of **computing** $h_{\Theta}(x)$ is called **forward propagation** (since we must start with the activations of the input units, and then we forward propagate these to compute the activations in the hidden layer and so on). (c.f back propagation, where we are given $h_{\Theta}(x)$ and want to learn the weights/parameters.)

Note. There is a Θ matrix for each layer l in the network, with $\Theta_{a_l, a_{l-1}}^{(l-1)}$ ($a_l :=$ index of activation node in layer l being computed, $a_{l-1} :=$ index of activation node in layer $l - 1$ being multiplied by).

Remark. Looking at how we compute each activation unit, $a_i^{(j)}$, we notice that what this neural network is just doing logistic regression (with “learned” inputs).

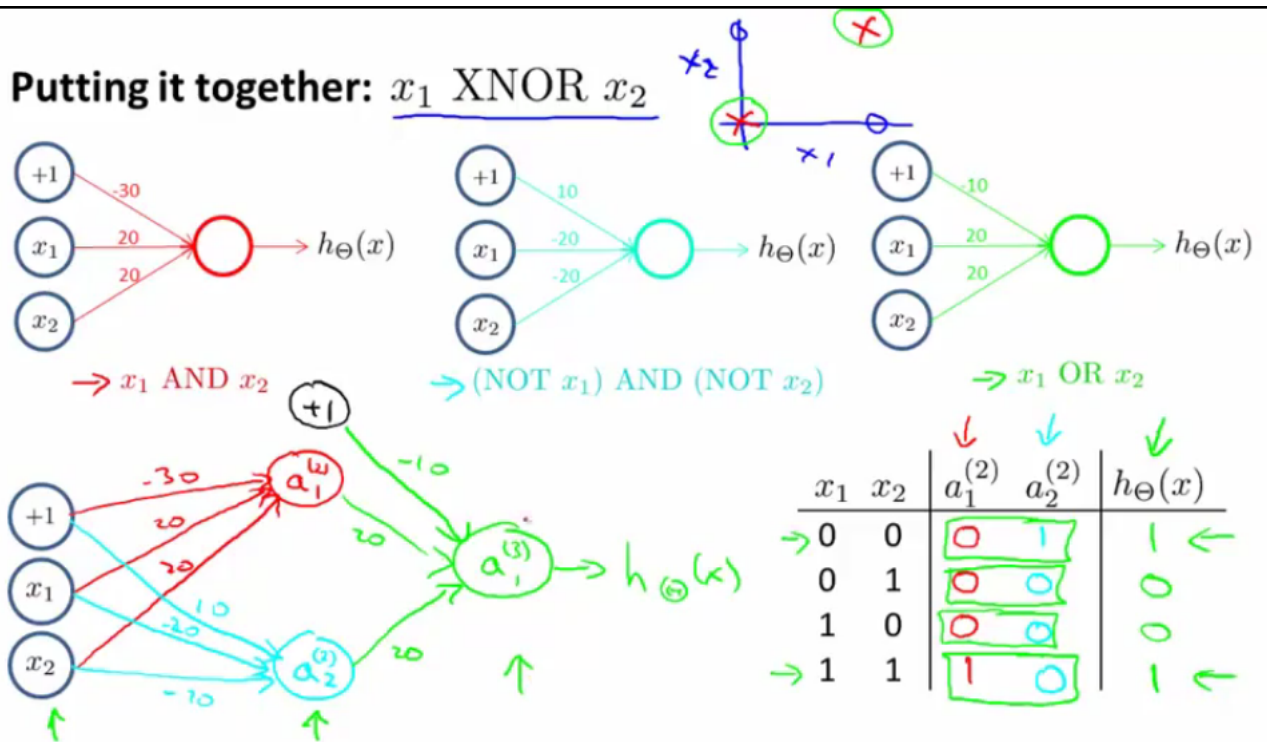


Figure 6.2: Neural network are used to learn more complex functions with each layer.

6.3 Multiple output units: One-vs-all

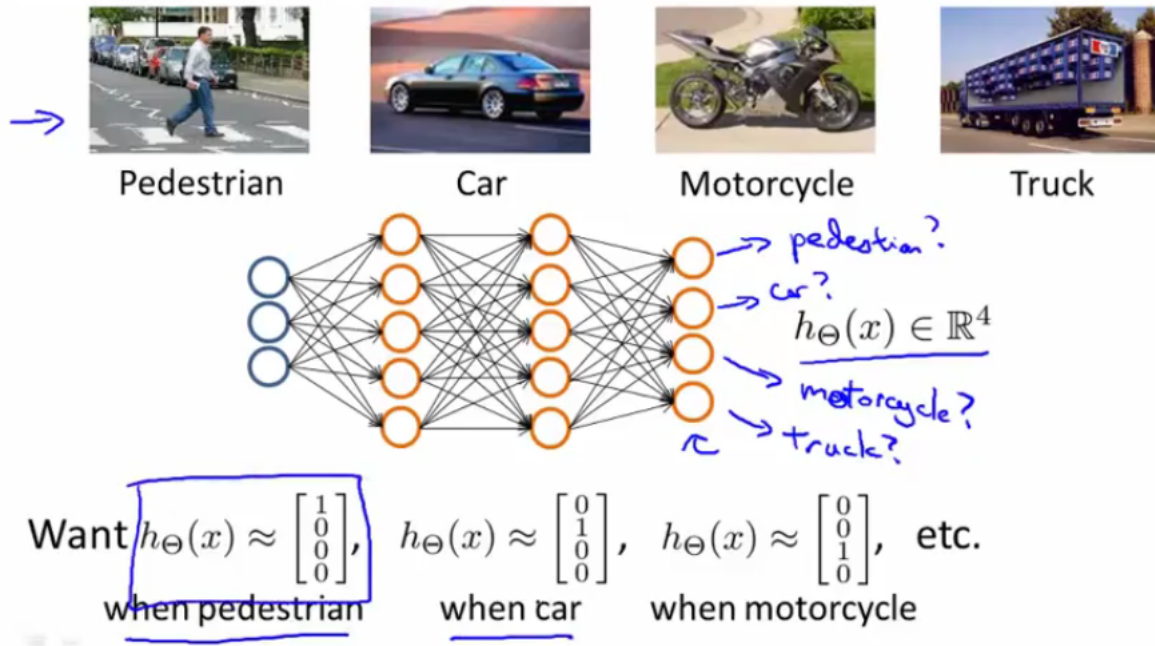


Figure 6.3: In the one vs. all (equal to 4 here) representation, instead of letting $y \in \{0,1\}$, we let $y \in \{[1, 0, 0, 0]^T, [0, 1, 0, 0]^T, [0, 0, 1, 0]^T, [0, 0, 0, 1]^T\}$.

6.4 Evaluation: Cost Function

Notation 2.

- L := total # layers in net work
- s_l := # units (excluding bias unit) in layer l
- s_L := # units in output layer
- K := # output units/classes

The cost function for neural networks is a generalisation of the cost function used from logistic regression (with regularisation); so $h_{\Theta}(x) \in \mathbb{R}^K$ (i.e. $(h_{\Theta}(x))_i$ = probability that the i^{th} output is 1), and we take the sum over these K output units in the cost function:

$$J(\Theta) = -\frac{1}{m} \left[\sum_{i=1}^m \sum_{k=1}^K y_k^{(i)} \log \left(h_{\Theta}(x^{(i)})_k \right) + \left(1 - y_k^{(i)} \right) \log \left(1 - \left(h_{\Theta}(x^{(i)})_k \right) \right) \right] + \frac{\lambda}{2m} \sum_{l=1}^{L-1} \sum_{i=1}^{s_l} \sum_{j=1}^{s_{l+1}} \left(\Theta_{ji}^{(l)} \right)^2$$

Remark. The first half of the cost function is saying (“average sum of logistic regression”)

- For each training data example $(1, \dots, m)$.
 - Some for each position in the output vector.

6.5 Optimisation: Stochastic gradient descent using backpropagation to compute the gradient.

To find $\min_{\Theta} J(\Theta)$ using gradient descent or one of the advanced optimisation algorithms, we need to compute $J(\Theta)$ and $\frac{\partial}{\partial \Theta_{ij}^{(l)}} J(\Theta)$ (recall $\Theta_{ij}^{(l)} \in \mathbb{R}$).

6.5.1 Gradient Computation for the case of one training example

Computing the gradient in the case of one training example (\mathbf{x}, \mathbf{y}) , we see that:

Given one training example (x, y) :

Forward propagation:

$$\begin{aligned}
 & \underline{a}^{(1)} = \underline{x} \\
 \rightarrow & \underline{z}^{(2)} = \underline{\Theta}^{(1)} \underline{a}^{(1)} \\
 \rightarrow & \underline{a}^{(2)} = g(\underline{z}^{(2)}) \quad (\text{add } \underline{a}_0^{(2)}) \\
 \rightarrow & \underline{z}^{(3)} = \underline{\Theta}^{(2)} \underline{a}^{(2)} \\
 \rightarrow & \underline{a}^{(3)} = g(\underline{z}^{(3)}) \quad (\text{add } \underline{a}_0^{(3)}) \\
 \rightarrow & \underline{z}^{(4)} = \underline{\Theta}^{(3)} \underline{a}^{(3)} \\
 \rightarrow & \underline{a}^{(4)} = \underline{h_{\Theta}(x)} = g(\underline{z}^{(4)})
 \end{aligned}$$

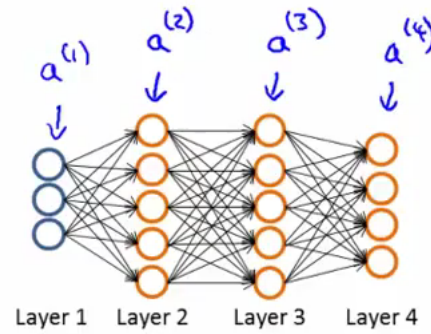


Figure 6.4: **Step 1 - Forward Propagation** (Calculating the activations $\underline{a}^{(i)}$)

This algorithm takes the initial input into that network and pushes the input through the network to the generation of an output hypothesis.

Gradient computation: Backpropagation algorithm

Intuition: $\underline{\delta}_j^{(l)}$ = "error" of node j in layer l .

For each output unit (layer $L = 4$)

$$\delta_j^{(4)} = \underline{a_j^{(4)}} - y_j \quad (\underline{h_{\Theta}(x)})_j \quad \delta^{(4)} = \underline{a^{(4)}} - \underline{y}$$

$$\rightarrow \delta^{(3)} = (\underline{\Theta}^{(3)})^T \delta^{(4)} \cdot * g'(\underline{z}^{(3)})$$

$$\delta^{(2)} = (\underline{\Theta}^{(2)})^T \delta^{(3)} \cdot * g'(\underline{z}^{(2)})$$

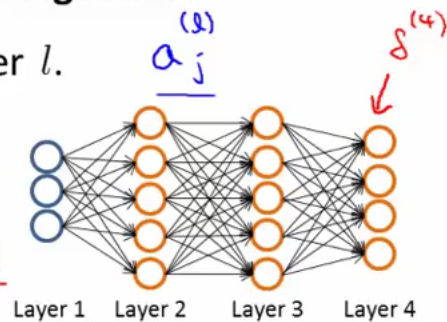


Figure 6.5: **Step 2 - Backpropagation** (Calculating the gradients $\underline{\delta}^{(i)}$)

This algorithm takes the output you got from your network, compares it to the real value y and calculates how wrong the network was (i.e. how wrong the parameters were). It then, using the error you've just calculated, back-calculates the error associated with each unit from the preceding layer (i.e. layer $L - 1$). These "error" measurements for each unit can be used to calculate the partial derivatives, which can then be used to calculate the partial derivative for gradient descent.

Note. The $*$ denotes element-wise multiplication.

Remark. We do not calculate $\underline{\delta}^{(1)}$ as the first layer does not have any error associated with it (it's just the features we observed in our training set).

Remark. When the cost function is **not** regularised (i.e. $\lambda = 0$), it can be shown that $\frac{\partial}{\partial \Theta_{ij}^{(l)}} J(\Theta) = a_j^{(l)} \delta_i^{(l+1)}$.

6.5.2 Gradient Computation for m training examples

For a training set $\{(x^{(1)}, y^{(1)}), \dots, (x^{(m)}, y^{(m)})\}$:

Algorithm 1. Backpropagation Algorithm

Set $\Delta_{ij}^{(l)} = 0, \forall l, i, j$ (i.e. this has each node as one dimension and each training data example as the other).

For $i = 1, \dots, m$:

Set $a^{(1)} = x^{(i)}$

Perform forward propagation to compute $a^{(l)}$ for $l = 2, 3, \dots, L$

Using $y^{(i)}$, compute $\delta^{(L)} = a^{(L)} - y^{(i)}$

Compute $\delta^{(L-1)}, \delta^{(L-2)}, \dots, \delta^{(2)}$

$\Delta_{ij}^{(l)} := \Delta_{ij}^{(l)} + a_j^{(l)} \delta_i^{(l+1)}$ (or vectorised form $\Delta^{(l)} := \Delta^{(l)} + \delta^{(l+1)} (a^{(l)})^T$)

$$D_{ij}^{(l)} := \begin{cases} \frac{1}{m} \Delta_{ij}^{(l)} + \lambda \Theta_{ij}^{(l)} & \text{if } j \neq 0 \\ \frac{1}{m} \Delta_{ij}^{(l)} & \text{if } j = 0 \end{cases}$$

Remark. For quite a complicate proof, it can be shown that the partial derivatives $\frac{\partial}{\partial \Theta_{ij}^{(l)}} J(\Theta) = D_{ij}^{(l)}$.

6.6 Backpropagation in practice

6.6.1 Unrolling parameters

With neural networks, we are working with sets of matrices:

$$\Theta_1, \Theta_2, \Theta_3, \dots; D_1, D_2, D_3, \dots$$

In order to use optimizing functions such as `fminunc()`, we need to "unroll" all the elements and put them into one long vector (MATLAB):

```
thetaVector = [ Theta1(:); Theta2(:); Theta3(:) ];
deltaVector = [ D1(:); D2(:); D3(:) ];
```

6.6.2 Gradient checking

Backpropagation has a lot of details. Small bugs can easily creep in so that it looks like $J(\Theta)$ is decreasing, but in reality it may not be decreasing by as much as it should.

We can approximate the derivative of our cost function, for some small $\varepsilon > 0$, as

$$\frac{\partial}{\partial \Theta} J(\Theta) \approx \frac{J(\Theta + \varepsilon) - J(\Theta - \varepsilon)}{2\varepsilon}$$

and for multiple theta matrices, we can approximate the derivative w.r.t. Θ_j as

$$\frac{\partial}{\partial \Theta_j} J(\Theta) \approx \frac{J(\Theta_1, \dots, \Theta_{j-1}, \Theta_j + \varepsilon, \Theta_{j+1}, \dots, \Theta_n) - J(\Theta_1, \dots, \Theta_{j-1}, \Theta_j - \varepsilon, \Theta_{j+1}, \dots, \Theta_n)}{2\varepsilon}$$

Remark. Andrew Ng typically uses $\varepsilon = 10^{-4}$.

Finally check that `gradApprox` \approx `deltaVector`.

Note. Once you've verified once that your backpropagation algorithm is correct, then you don't need to compute `gradApprox` again. The code to compute `gradApprox` is very slow.

6.6.3 Random initialisation

Initializing all theta weights to 0 does not work with neural networks. When we backpropagate, all nodes will update to the same value repeatedly. Thus we use **random initialization**, which serves the purpose of symmetry breaking.

Initialise each $\Theta^{(l)} \in \mathbb{R}^{n_{l-1}, n_l}$ (where $n_l := \#$ neurons in layer l (I WORKED THIS OUT LATE - CHECK)) to a random value between $[-\varepsilon, \varepsilon]$ with

$$\varepsilon = \frac{\sqrt{6}}{\sqrt{n_l + n_{l-1}}}$$

E.g. $\Theta^{(1)} = \text{rand}(n_{l-1}, n_l) * 2\varepsilon - \varepsilon \in \mathbb{R}^{n_{l-1}, n_l}$ (where the `rand` function produces a $n_{l-1} \times n_l$ matrix).

6.7 Implementation summary and some best practices of using neural networks for machine learning

1. **REPRESENTATION:** Pick a network architecture, including how many hidden units there are in each layer and how many layers in total.
 - (a) The higher the # hidden units per layer is usually produces more accurate results, but we must take into account the computation cost.
 - (b) # hidden layers :
 - i. "1 hidden layer is sufficient for the large majority of problems".
 - ii. If the data **linearly separable**, then you **don't need any hidden** layers at all.
 - iii. DNN=more than 3; most papers on deep learning use networks with 5-7 layers.
 - iv. Geoff Hinton: "Add layers until you overfit (if you're not overfitting, your network isn't big enough.). Then add dropout or another regularization method."
 - (c) # neurons for each layer:
 - i. Roughly same for all hidden layers and usually at 1 to 3 times the input variables (or mean of the # input and # output nodes).
 - ii. Yoshia Bengio: "It is a hyper-parameter to be optimized, as usual."
 - iii. WARNINGS:
 - A. **Too few nodes** will lead to high error for your system as the predictive factors might be too complex for a small number of nodes to capture.
 - B. **Too many nodes** will overfit to your training data and not generalise well.
 - (d) # input units = dimension of features $x^{(i)}$; # output units = # classes
2. **EVALUATION:** Randomly initialise the weights (as discussed above).
3. **EVALUATION:** Implement forward propagation to get $h_{\theta}(x^{(i)})$.
4. **EVALUATION:** Compute the cost function
5. **EVALUATION:** Implement back propagation to compute partial derivatives.

```
for i = 1:m {  
    Forward propagation on (xi, yi) --> get activation (a) terms  
    Back propagation on (xi, yi) --> get delta (δ) terms  
    Compute Δ := Δ1 + δ1+1(a1)T  
}
```

With this done compute the partial derivative terms

Figure 6.6: Backpropagation is usually done with a for loop over training examples, like above. It can be done without a for loop, but this is much more complicated way of doing things.

- (a)
 - (b) Use gradient checking to confirm your back propagation works. Then disable gradient checking.
6. **OPTIMISATION:** Use gradient descent or a built-in optimization function to minimize the cost function with the weights in theta.
 - (a) If $J(\Theta)$ is not convex, then some algorithms can be susceptible to local minimum. In practice this is not usually a huge problem, but we can't guarantee programs with find global optimum should find good local optimum at least.

6.7.1 Dealing with overfitting

- The easiest and most common method to reduce overfitting on image data is to artificially enlarge the dataset using label-preserving transformations (e.g. by flipping the image, rotating it slightly, removing some of the image).