MATH 567: Introduction to Data Mining and Analysis
Introduction to Neural networks

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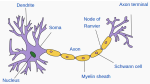
This lecture is based on the UFLDL tutorial (http://deeplearning.stanford.edu/)

Neurons



Neuron representation (Source: Wiki).

- Our brain contains about 86 billion neurons.
- Each neuron receives signals from other neurons via its many dendrites (input).
- Each neuron has a single axon (output).
- Neuron make on average 7,000 synaptic connections.
- Signals are sent via an electrochemical process.
- When a neuron fires, it starts a chain reaction that propagates information.
- There are *excitatory* and *inhibitory* synapses.

See Izenman (2013) for more details.

Neurons (cont.)

- Our brain *learns* by changing the **strengths** of the connections between neurons or by **adding** or **removing** such connections.
- Relating brain networks to *functions* is still a very challenging problem.
- Constructing a "universal" learning machine/algorithm?
- In some sense, no machine learning algorithm is universally better than any other (Goodfellow et al., "Deep learning"):

Theorem: (No free lunch theorem) (Wolpert, 1996) Averaged over all possible data generating distributions, every classification algorithm has the same error rate when classifying previously unobserved points.

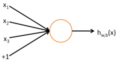
- Still, there is hope to construct an *algorithm* that performs well at many tasks (e.g. the human brain).

Neural networks:

- **Inspired** by neuroscience (probably very far from real neurons).
- Use multiple layers of neurons to represent data.
- Very popular in computer vision, natural language processing, and many other fields.
- Today, neural network models are often called *deep learning*.

Neural networks

Single neuron model:



Source: UFLDL Tutorial

Input: x_1, x_2, x_3 (and $+1$ intercept).
Output: $h_{W,b}(x) = f(W^T x) = f(W_1 x_1 + W_2 x_2 + W_3 x_3 + b)$,
where f is the *sigmoid* function:

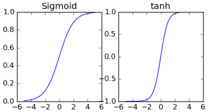
$$f(x) = \frac{1}{1+e^{-x}}.$$

Other common choice for f:

$$f(x) = \tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}.$$

Neural networks (cont.)

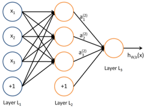
The function f acts as an **activation** function.



Idea: Depending on the input of the neuron and the *strength* of the links, the neuron "fires" or not.

Neural network models

A **neural networks model** is obtained by hooking together many neurons so that the output of one neuron becomes the input of another neuron.



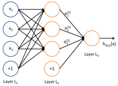
Source: UFLDL tutorial

Note: Each layer includes an intercept "$+1$" (or bias unit)

- Leftmost layer = input layer.
- Rightmost layer = output layer.
- Middle layers = hidden layers (not observed).

We will let n_l denote the **number of layers** in our model ($n_l = 3$ in the above example).

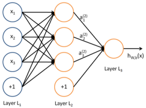
Notation



- n_l = number of layers.
- We denote the layers by $L_1, \dots, L_{n_l}$, so L_1 = input layer and L_{n_l} = output layer.
- $W_{ij}^{(l)}$ = weight associated with the connection between unit j in layer l, and unit i in layer $l+1$. (Note the order of the indices.)
- $b_i^{(l)}$is the bias associated with unit i in layer $l+1$.

In above example: $(W, b) = (W^{(1)}, b^{(1)}, W^{(2)}, b^{(2)})$. Here $W^{(1)} \in \mathbb{R}^{3\times 3}$, $W^{(2)} \in \mathbb{R}^{1\times 3}$, $b^{(1)} \in \mathbb{R}^3$, $b^{(2)} \in \mathbb{R}$.

Activation



- We denote by $a_i^{(l)}$ the **activation** of unit i in layer l.
- We let $a_i^{(1)} = x_i$ (input).

We have:

$$\begin{aligned}
a_1^{(2)} &= f(W_{11}^{(1)}x_1 + W_{12}^{(1)}x_2 + W_{13}^{(1)}x_3 + b_1^{(1)}) \\
a_2^{(2)} &= f(W_{21}^{(1)}x_1 + W_{22}^{(1)}x_2 + W_{23}^{(1)}x_3 + b_2^{(1)}) \\
a_3^{(2)} &= f(W_{31}^{(1)}x_1 + W_{32}^{(1)}x_2 + W_{33}^{(1)}x_3 + b_3^{(1)}) \\
h_{W,b} = a_1^{(3)} &= f(W_{11}^{(2)}a_1^{(2)} + W_{12}^{(2)}a_2^{(2)} + W_{13}^{(2)}a_3^{(2)} + b_1^{(2)}).
\end{aligned}$$

Compact notation

- In what follows, we will let $z_i^{(l)}$ = total weighted sum of inputs to unit i in layer l (including the bias term):

$$z_i^{(l)} := \sum_j W_{ij}^{(l-1)} a_j^{(l-1)} + b_i^{(l-1)} \qquad (l \geq 2).$$

- Note that that $a_i^{(l)} = f(z_i^{(l)})$.
- For example:

$$z_i^{(2)} = \sum_{j=1}^{3} W_{ij}^{(1)} x_j + b_i^{(1)} \qquad i = 1, 2, 3.$$

We extend f *elementwise*: $f([v_1, v_2, v_3]) = [f(v_1), f(v_2), f(v_3)]$.
Using the above notation, we have:

$$\begin{aligned} z^{(2)} &= W^{(1)} x + b^{(1)} \\ a^{(2)} &= f(z^{(2)}) \\ z^{(3)} &= W^{(2)} a^{(2)} + b^{(2)} \\ h_{W,b} &= a^{(3)} = f(z^{(3)}). \end{aligned}$$

Forward propagation

The previous process is called the **forward propagation** step.

- Recall that we defined $a^{(1)} = x$ (the input).
- The forward propagation can therefore be written as:

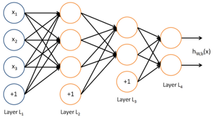
$$\begin{aligned} z^{(l+1)} &= W^{(l)} a^{(l)} + b^{(l)} \\ a^{(l+1)} &= f(z^{(l+1)}). \end{aligned}$$

Using matrix-vector operations, we can take advantage of fast linear algebra routines to quickly perform calculations in our network.

- Can use different **architectures** (i.e., pattens of connectivity between neurons).
- Typically, we use multiple densely connected layers.
- In that case, we obtain a **feedforward neural network** (no directed loops or cycles).

Multiple outputs

Neural networks may also have multiple outputs:



Source: UFLDL tutorial

- To train this network, we need observations $(x^{(i)}, y^{(i)})$ with $y^{(i)} \in \mathbb{R}^2$.
- Useful for applications where the output is multivariate (e.g. medical diagnosis application where output is whether or not a patient has a list of diseases).
- Useful to *encode* or *compress* information.

The universal approximation theorem

- What kind of functions can we approximate with neural networks?
- The following result shows that neural networks have a "universal" approximation property.

Theorem: (Cybenko, 1989) A single layer feedforward neural network can uniformly approximate any continuous function defined on a compact subset K of $\mathbb{R}^n$.

- A subset of $\mathbb{R}^n$ is *compact* if it is closed ($x_n \in K$ and $x_n \to x$ implies $x \in K$) and bounded ($\|x\| \leq C$ for all $x \in K$).

Example: Let f be any continuous function defined on the unit cube $[0,1]^3$. Then for every $\epsilon > 0$, there exists a feedforward neural network $f_{W,b}$ with one layer such that

$$|f(x) - f_{W,b}(x)| < \epsilon \qquad \forall x \in [0,1]^3.$$