(Feed-Forward) Neural Networks

KGA

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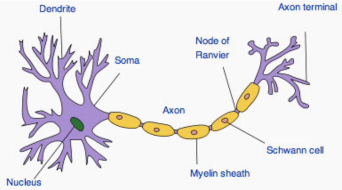
Outline

- In the previous lectures we have learned about tensors and factorization methods.
- RESCAL is a bilinear model for SRL that can be formulated as tensor factorization problem.
- Furthermore, we learned about optimization techniques which can be applied for learning score-based models.
- Today we will learn about a new class of algorithms which can be applied for SRL, namely neural networks.
- We will see how to apply them for SRL in the following lecture.

Artificial Neurons



source: Wikipedia

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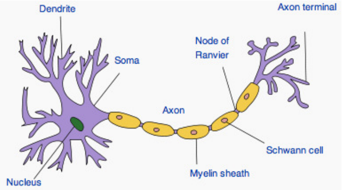

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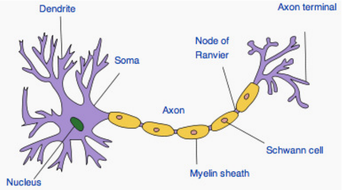

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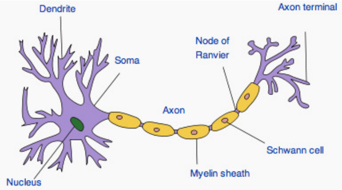

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  Basic idea: reduce the neuron to its essentials.

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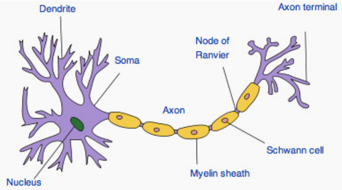

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- Neurons are connected to each other with synapses. Thus, they form a network. This complicates things even more.
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  Basic idea: reduce the neuron to its essentials.
- There are a number of greatly simplified neuron models. One of the simplest models is by McCulloch and Pitts.

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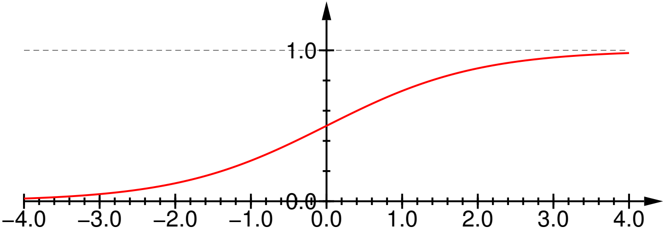
- The weight is positive for excitatory and negative for inhibitory connections.
- The absolute value of the weight is small for weak connections and large for strong connections.

Artificial Neurons

When the neuron's membrane potential exceeds a threshold then the neuron emits a spike (which can propagate to multiple receivers) and resets its membrane potential. The spike frequency as a function of the incoming power is a non-linear **transfer function** (also simply called **non-linearity**):



We call such a function a **sigmoid** or **sigmoidal function**. The standard formula is

$$\nu = \sigma(u) = \frac{1}{1 + e^{-u}} \quad .$$

Artificial Neurons

- Now assume we have a pool of neurons, numbered $1, \ldots, n$. Let u_i be the membrane potential and ν_i be the firing rate of neuron number i, and let w_{ji} be the synaptic weight of the connection from i to j (which is zero if the neurons are not connected).

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- This model draws inspiration from biology. However, it is so abstract that in the end it has little in common with its biological counterpart. It should rather be viewed as a computational unit in a mathematical learning machine.

Artificial Neurons

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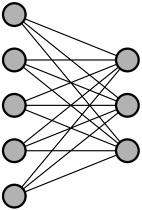
- Usually many neurons process the input, so we have multiple Perceptrons in parallel:



Layered Neural Networks

- Let $\nu^{(0)} \in \mathbb{R}^m$ denote the vector of firing rates coming from the inputs (sensors, data), and let $\nu^{(1)} \in \mathbb{R}^n$ denote the vector of firing rates of the neurons. Let $W \in \mathbb{R}^{n \times m}$ be the matrix with entries w_{ji}. Also, let σ denote the component-wise application of the transfer function.

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- The computation can be written in compact form:

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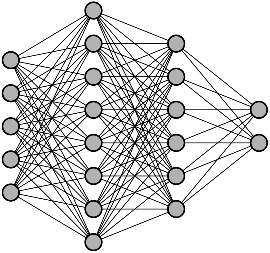
- Neurons can not only receive input from sensors, but also from other neurons. What if we feed the outputs into another layer of neurons?

Layered Neural Networks

- The resulting architecture is called a (layered) feed-forward neural network, or multi layer Perceptron (MLP).



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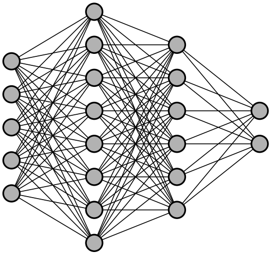

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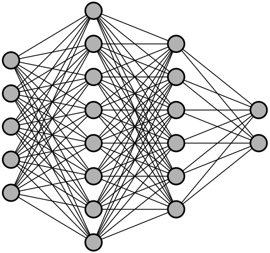

- This example network has an **input layer** with 5 nodes, two **hidden layers** with 8 and 6 neurons, and an **output layer** with 2 neurons.
- The size of the input and output layers is determined by the problem (dimension of the vectors x and y), but number and size of the hidden layers is arbitrary.

Layered Neural Networks

- Now let $\nu^{(0)}$ denote the vector of inputs, let $\nu^{(i)}$ denote the vector of firing rates in layer i, and let $W^{(i)}$ denote the matrix of connections from layer $i-1$ to layer i. Then we have the overall model:

$$\nu^{(n)} = \sigma_{\text{out}}\left(W^{(n)} \cdot \sigma\Big(W^{(n-1)} \cdot \sigma\big(\dots \sigma(W^{(1)} \cdot \nu^{(0)}) \dots \big)\Big)\right) \ .$$

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- This is effectively the same as embedding affine functions into

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- The non-linearities are not adaptive, but they are nevertheless important! Without them the model would collapse into the linear map $W = W^{(n)} \cdot \ldots \cdot W^{(1)}$. Then all computations were linear.
- It turns out that a neural network with sigmoid transfer functions is indeed far more powerful than a linear model. In a sense, it can compute "everything".

Universal Approximation Property

Theorem. Let $\sigma : \mathbb{R} \to \mathbb{R}$ be a continuous, non-constant, bounded, and monotonically increasing function. Let $K \subset \mathbb{R}^m$ be compact, and let $\mathcal{C}(K)$ denote the space of continuous functions $K \to \mathbb{R}$. Then, given a function $g \in \mathcal{C}(K)$ and an accuracy $\varepsilon > 0$, there exists a hidden layer size $N \in \mathbb{N}$ and a set of coefficients $w_i^{(1)} \in \mathbb{R}^m$, $w_i^{(2)}, b_i \in \mathbb{R}$ (for $i \in \{1, \ldots, N\}$), such that

$$f : K \to \mathbb{R} ; \quad f(x) = \sum_{i=1}^{N} w_i^{(2)} \cdot \sigma\Big((w_i^{(1)})^T x + b_i \Big)$$

is an ε-approximation of g, that is,

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Corollary. Neural networks with a single sigmoidal hidden layer and linear output layer are universal approximators.

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- A network with fixed layer sizes can only model a subspace of all continuous functions. Its dimensionality is limited by the number of weights.
- The continuous functions form an infinite dimensional vector space. Therefore arbitrarily large hidden layer sizes are needed.
- The universal approximation property is not as special as it seems. For example, polynomials are universal approximators (Weierstraß theorem).

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- **Auto-encoders, (restricted) Boltzmann machines**, and **self-organizing maps** are used for unsupervised learning

Other Neural Networks

In this lecture we cover only feed-forward neural networks, because this is the most basic and most relevant class for supervised (and unsupervised) learning and the class applied to SRL. A broad range of other network types has been developed.

- The linear+sigmoid processing model can be replaced by other functions. For example, this leads to radial basis function models.
- **Convolutional Neural Networks (CNNs)** are inspired by the organization of the animal visual cortex. Each neuron receives input only from a "local patch" (corresponding to the receptive field in real neurons).
- Synapses can form loops. This requires the introduction of time delays. Then we speak of **Recurrent Neural Networks (RNNs).** These are even more powerful models: they are not simple mappings, but stateful computers.
- **Auto-encoders, (restricted) Boltzmann machines**, and **self-organizing maps** are used for unsupervised learning

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- This is in rough correspondence with our understanding of how the visual cortex processes images.
- Recently deep learning revolutionized a lot of fields like image and language procession, machine translations etc. It was also part of Alpha-Go.

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- However, this is not helpful in practice. It does not tell us how to actually set the network size, let alone the weights.
- Until now we have defined neural networks as a class of models. We do not have a learning rule yet.
- Neural networks are trained based on **stochastic gradient descent** as described in the following.

(Online) Steepest Descent Training

- Let w denote a vector collecting all weights of a neural network. This is a "linearized" version of all of its weight matrices.

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denote the error of the network, as a function of the weights.
- The sum may run over the whole data set ($|S| = n$, batch mode), over small subsets ($|S| \ll n$, mini batches), or only over a single example ($|S| = 1$, online mode).

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- This is usually what we want when training a neural network. So why care about online and mini batch errors?
- The reason is that the online error is much faster to compute, namely by a factor of n (size of the data set). Thus its use allows for many more gradient descent steps.

(Online) Steepest Descent Training

- Assume we have computed the gradient of the error $\nabla_w E(w)$ with respect to the weights. Then we can perform a step of gradient descent with learning rate η to update the wights.

$$w \leftarrow w - \eta \cdot \nabla_w E(w) \ .$$

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- We write this error as

$$E(w) = L\left(\sigma\left(W^{(n)} \cdot \sigma\left(W^{(n-1)} \cdot \sigma\left(\ldots W^{(1)} \cdot x \ldots\right)\right)\right), y\right) \ ,$$

  where $W^{(k)}$ are the weight matrices and σ is the component-wise non-linearity.

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  where $W^{(k)}$ are the weight matrices and σ is the component-wise non-linearity.
- The gradient can be calculated by the chain rule.
- **Backpropagation** is an algorithm for doing this fast. It will be introduced in the next lecture.

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Acknowledgments

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