CS 584 – Machine Learning

Topic: Neural Networks

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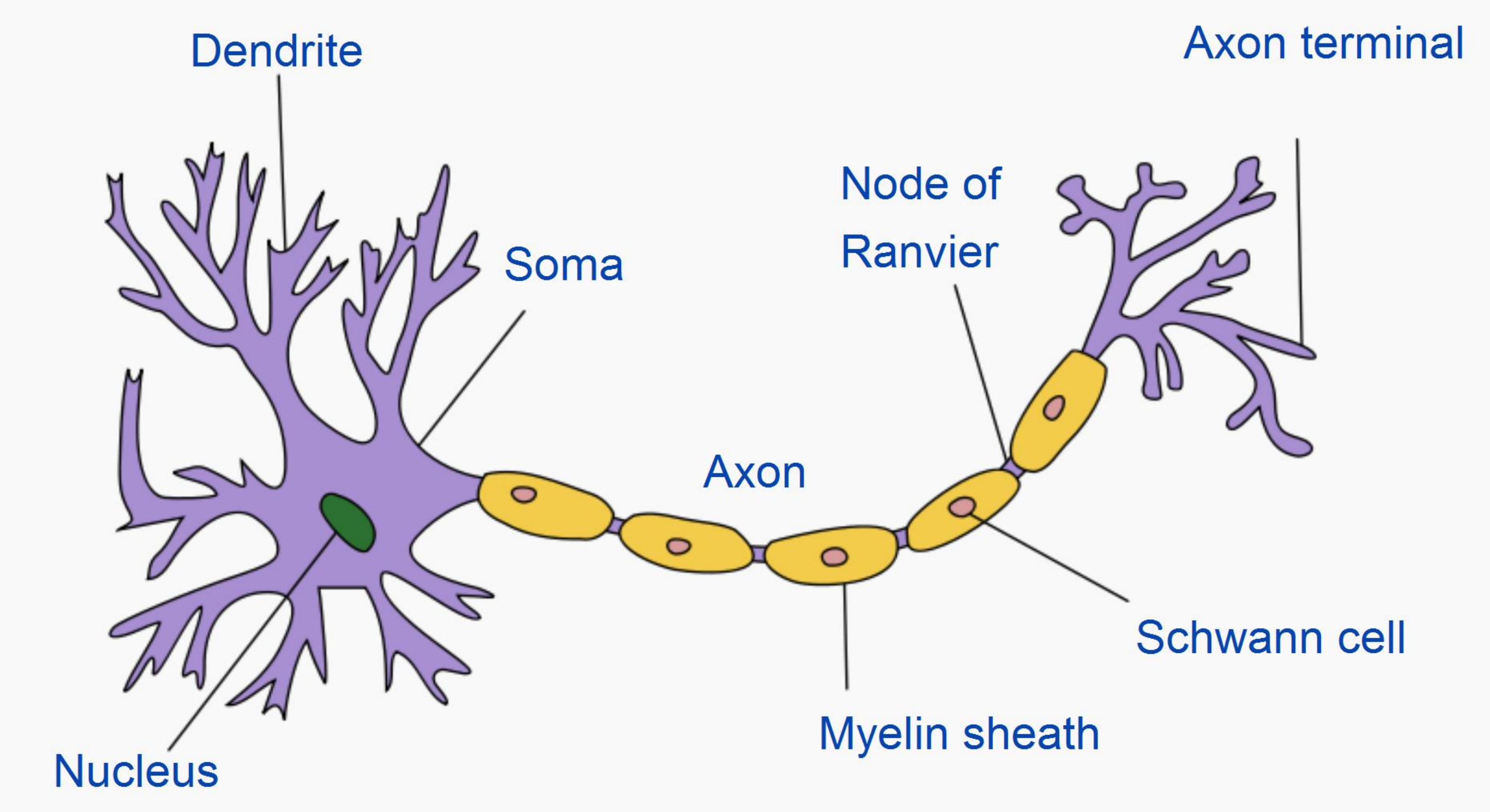
Neuron



Dendrite
Axon terminal
Node of Ranvier
Soma
Axon
Schwann cell
Myelin sheath
Nucleus

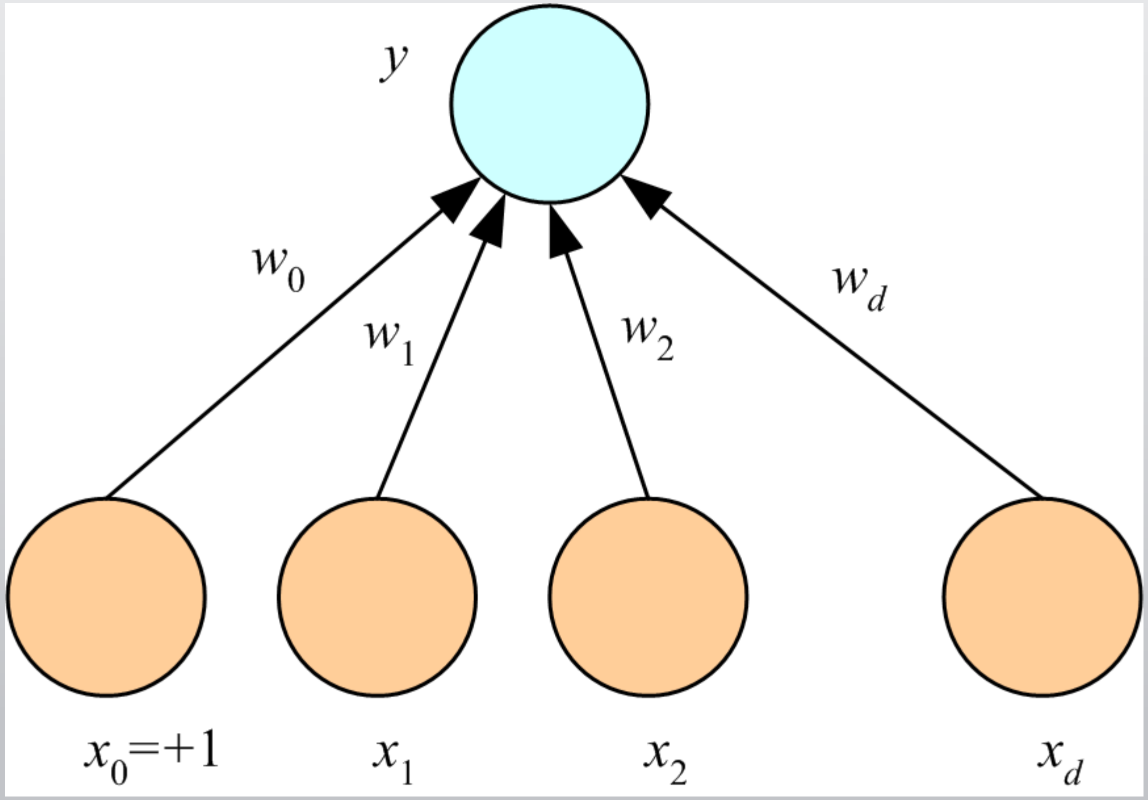
Neuron

- Neurons can have multiple dendrites and at most one axon
- Typical connections are from an axon of a neuron to dendrites of other neurons
- Synaptic signals are received through dendrites and somas; signals are transmitted through axons
- Signals can excite or inhibit the receiving neuron
- A neuron fires when the excitement is above a threshold
- Note: these are general statements and simplifications, and there are many exceptions!

Artificial Neural Networks

- Artificial neural networks are *inspired* by real neurons
- 1943 – One of the first neural computational models was proposed by McCulloch and Pitts
- 1958 – Rosenblatt proposed perceptron
- 1969 – A paper by Minsky and Papert almost killed the entire field
  - Perceptrons are incapable of representing XOR
  - Computational resources are too great
- 1975 – Backpropagation algorithm renewed interest in neural networks
- 1980s – parallel architectures were popular
- Late 1990s and 2000s – other methods, such as support vector machines, became more popular
- 2010s – neural networks of several hidden layers are back with the new name "deep learning"

Perceptron



$$y = sign(w_0 + \sum w_i x_i)$$

What an Artificial Neuron Does

- Takes a weighted sum of its inputs
  - $w_0 + \sum_{i=1}^{k} w_i x_i$
  - Assume that there is always a constant input 1, that is, $x_0 = 1$. Then,
  - $\sum_{i=0}^{k} w_i x_i$
- Passes this sum through its activation function
  - $f\left(\sum_{i=0}^{k} w_i x_i\right)$

EXAMPLES

- Logical AND
- Logical OR
- Logical XOR
- See OneNote and Notebook

Simple Multilayer Network for XOR

- $XOR(A, B) = (A \land \neg B) \lor (\neg A \land B)$
- One perceptron for $(A \land \neg B)$
- One perceptron for $(\neg A \land B)$
- One perceptron for combining the outputs, through OR, of the two previous perceptrons
- See Notebook

VARIOUS ACTIVATION FUNCTIONS

- Identity function
- Bipolar step function
- Binary sigmoid
- Bipolar sigmoid
- Hyperbolic tangent

Bipolar Step Function

- $f\left(\sum_{i=0}^{k} w_i x_i\right) = sign\left(\sum_{i=0}^{k} w_i x_i\right)$
- Returns either +1 or -1 (except right on the decision boundary)
- Useful for both hidden layers and output layer
- However, its discontinuous and it is problematic for learning algorithms that require taking its derivative

Identity Function

- $f\left(\sum_{i=0}^{k} w_i x_i\right) = \sum_{i=0}^{k} w_i x_i$
- Typically used for the output neurons, when the task is regression
- The identity function should not be used in the hidden layers
  - Linear combination of linear functions is another linear function, and hence using the identity function in the hidden layers do not increase representative power of the neural network

Binary Sigmoid

- $f\left(\sum_{i=0}^{k} w_i x_i\right) = \frac{1}{1+e^{-\sum_{i=0}^{k} w_i x_i}}$

$\frac{1}{1+e^{-s}}$

- This is the logistic function that we used
  - Except, notice the minus sign in front of the sum
    - This is only a convention and does not change much
- The output of the binary sigmoid is between 0 and 1
  - Useful for output layer when the task is classification
  - The output can be interpreted as a probability

Hyperbolic Tangent

$$\frac{e^s - e^{-s}}{e^s + e^{-s}}$$

- $f\left(\sum_{i=0}^{k} w_i x_i\right) = \dfrac{e^{\sum_{i=0}^{k} w_i x_i} - e^{-\sum_{i=0}^{k} w_i x_i}}{e^{\sum_{i=0}^{k} w_i x_i} + e^{-\sum_{i=0}^{k} w_i x_i}}$
- The output of tanh is between -1 and +1
  - Useful for output layer when the task is classification
  - Useful for both hidden and output layers

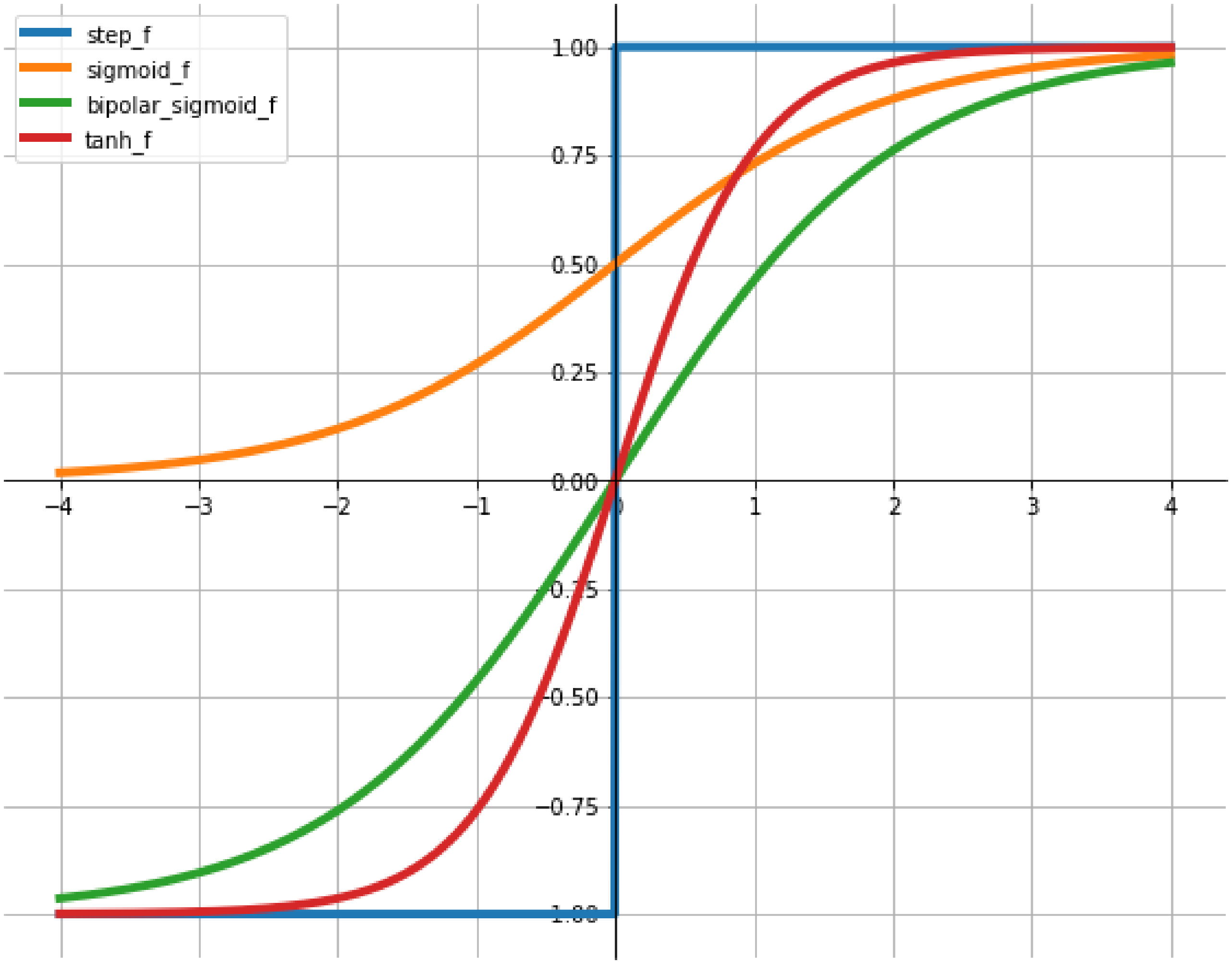
Relu

- $f\left(\sum_{i=0}^{k} w_i x_i\right) = \sum_{i=0}^{k} w_i x_i$ if $\sum_{i=0}^{k} w_i x_i > 0$;
  - 0 otherwise
- Typically used for hidden layers, especially for computer vision tasks

Bipolar Sigmoid

- $f\left(\sum_{i=0}^{k} w_i x_i\right) = \frac{2}{1+e^{-\sum_{i=0}^{k} w_i x_i}} - 1$
- This is a rescaled version of the binary sigmoid
- The output of the bipolar sigmoid is between -1 and +1
  - Useful for output layer when the task is classification
  - Useful for both hidden and output layers

Activation Function Plots



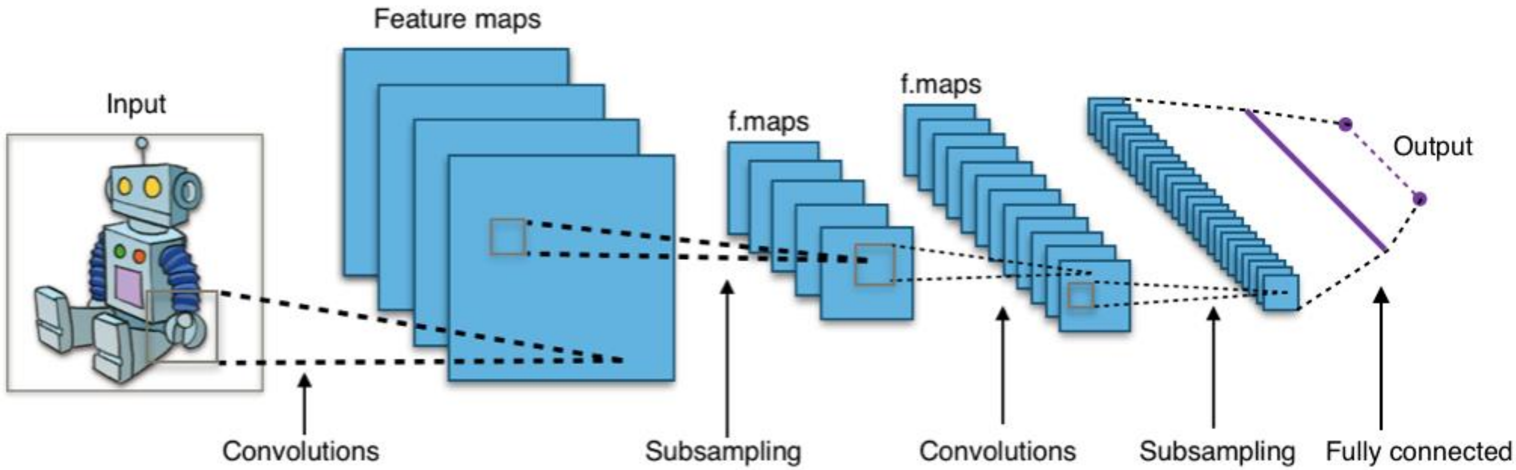
Deep Learning

- Several hidden layers structure
  - Millions of parameters
- Big data, big computation
- If a neural network with a single hidden layer is a universal approximator, why go deep?
  - "Why and When Can Deep -- but Not Shallow -- Networks Avoid the Curse of Dimensionality: a Review" https://arxiv.org/abs/1611.00740

Example DL Network Architectures

- Convolutional neural networks (CNN)
- Recurrent neural networks (RNN)
  - Long Short-Term Memory networks (LSTM)

Convolutional Neural Networks



https://commons.wikimedia.org/wiki/File:Typical_cnn.png

Convolution

+1	-1	+1

— Kernel

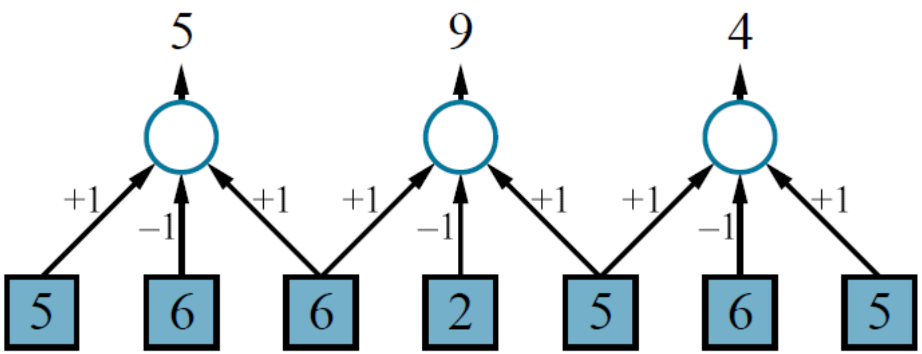


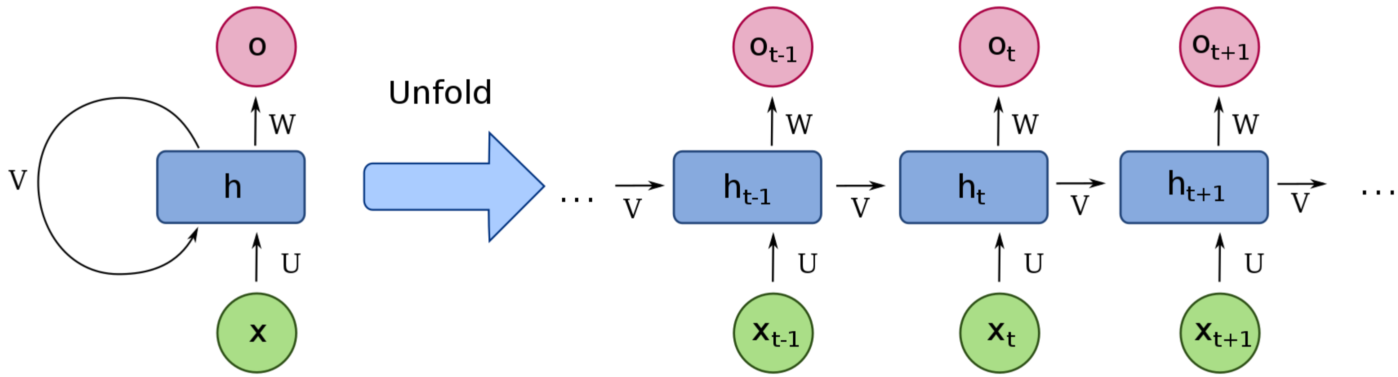
Figure 21.4 An example of a one-dimensional convolution operation with a kernel of size $l = 3$ and a stride $s = 2$. The peak response is centered on the darker (lower intensity) input pixel. The results would usually be fed through a nonlinear activation function (not shown) before going to the next hidden layer.

Figure from http://aima.cs.berkeley.edu/figures.pdf

Pooling

- Aggregates a set of adjacent units
- Like convolution, has a kernel size and a stride size
- Unlike convolution, weights are fixed (not learned)
- Examples
  - Average pooling
  - Max pooling

Recurrent Neural Networks



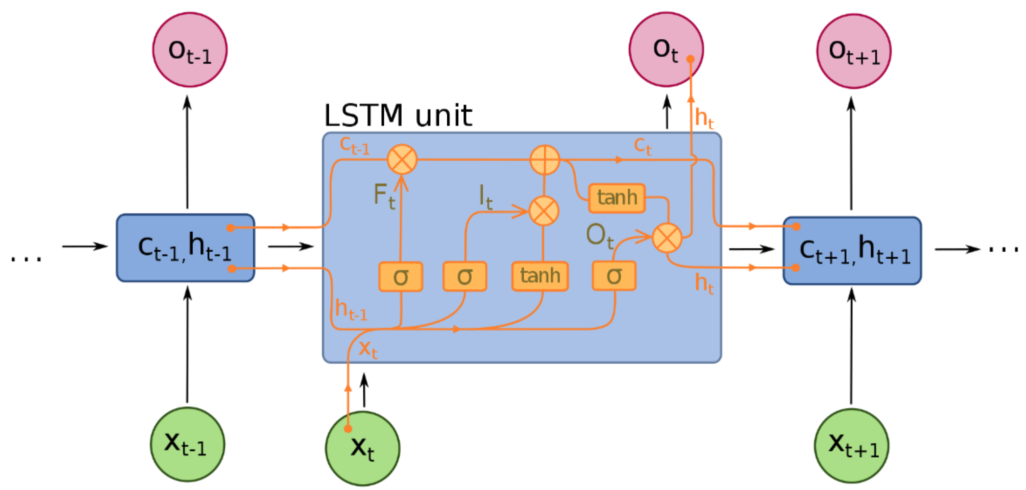
https://commons.wikimedia.org/wiki/File:Recurrent_neural_network_unfold.svg

The machine learning class is ....

'It'

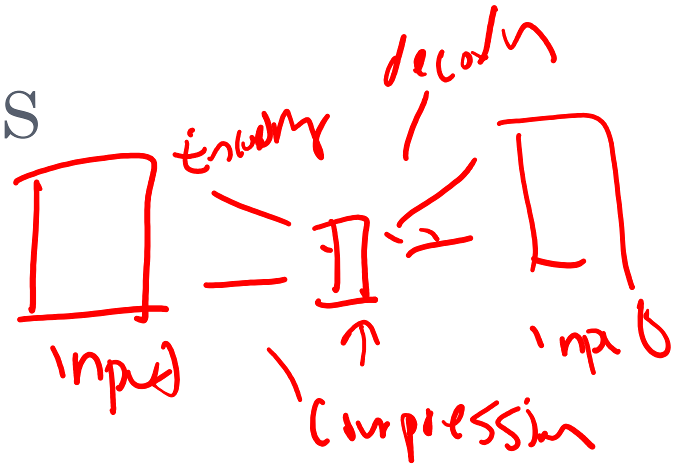
LONG SHORT-TERM MEMORY (LSTM)

- A specialized RNN
- Works better than vanilla RNN for "remembering" long sequences
- Has additional units
  - Cell, forget gate, input gate, output gate



https://commons.wikimedia.org/wiki/File:Long_Short-Term_Memory.svg

OTHER NETWORKS/CONCEPTS



- Autoencoder
  - Input and output are the same
- Deep autoregressive model
  - Predict an element of the data using the other elements
- Generative adversarial networks (GAN)
  - A pair of generator and discriminator networks

Learning the Weights

- Define an error (loss) function
- Take its derivative with respect to the weights
- Perform gradient descent

Some Error/Loss Functions

- Classification: log-loss, cross entropy, negative CLL
  - $-(1-t) \times ln(1-y) - t \times ln(y)$ = − CLL
  - t: the true target value (0/1)
  - y: probability of class 1
- Regression: squared error
  - $\frac{1}{2}(t-y)^2$
  - t: the true target value
  - y: the predicted value

BACKPROPAGATION ALGORITHM

- See OneNote

Derivatives of the Activation Functions

- f is the activation function, h is the weighted sum of the incoming signals
- $f(h(x)) \equiv$ binary sigmoid
  - $\frac{\partial f(h(x))}{\partial x} = f(h(x)) \times \left(1 - f(h(x))\right) \times \frac{\partial h(x)}{\partial x}$
- $f(h(x)) \equiv$ tanh
  - $\frac{\partial f(h(x))}{\partial x} = \left(1 + f(h(x))\right) \times \left(1 - f(h(x))\right) \times \frac{\partial h(x)}{\partial x}$
- See OneNote

Overfitting

- Neural networks are powerful tools
- Even with a single hidden layer, they are "universal approximators", i.e., they can approximate arbitrary functions arbitrarily close
- Therefore, it is very easy to overfit them
- To prevent overfitting, utilize
  - Domain knowledge
  - Shared parameters
  - Validation data
  - Regularization
  - Dropout

Some Libraries

- Scikit-learn
  - https://scikit-learn.org/stable/modules/neural_networks_supervised.html
  - Only MLP; no GPU support
- Keras
  - https://keras.io/
- Tensorflow
  - https://www.tensorflow.org/
- PyTorch
  - https://pytorch.org/