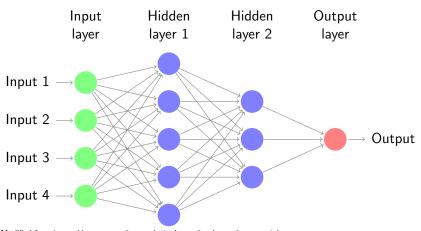
Neural networks Architectures and training tips

Sebastian Björkqvist

IPRally Technologies

09.01.2019

What is a neural network?



Modified from http://www.texample.net/tikz/examples/neural-network/

What is a neural network?

At each hidden layer node i the output value is calculated by

$$o_i = \sigma(\sum w_{ki}o_{ki-1} + b_i).$$

What is a neural network?

At each hidden layer node i the output value is calculated by

$$o_i = \sigma(\sum w_{ki}o_{ki-1} + b_i).$$

The function σ is called the activation function. It must be non-linear to allow the network to learn non-linear dependencies.

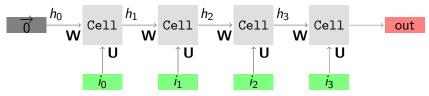
■ Can approximate any function [Hornik, 1991]

- Can approximate any function [Hornik, 1991]
- May learn to respond to unexpected patterns

- Can approximate any function [Hornik, 1991]
- May learn to respond to unexpected patterns
- Useful especially when the amount of data is large

- Can approximate any function [Hornik, 1991]
- May learn to respond to unexpected patterns
- Useful especially when the amount of data is large
- Less need for feature engineering compared to traditional ML methods

Recurrent neural network (RNN)



Processes each element of the input sequence in order, and keeps information about the past elements in a hidden state vector.

Recurrent neural network (RNN)

At each timestep t the new hidden state is calculated using the new input at this timestep and the existing hidden state. The most basic version is the following:

$$h_t = \sigma(Wh_{t-1} + Ui_t + b).$$

Recurrent neural network (RNN)

At each timestep t the new hidden state is calculated using the new input at this timestep and the existing hidden state. The most basic version is the following:

$$h_t = \sigma(Wh_{t-1} + Ui_t + b).$$

Other RNN architectures (for instance LSTM or GRU) use more complicated ways of updating the hidden state to control the flow of information to and from the hidden state.

+ Accepts input of variable size, i.e. sequences (time series, sentences etc)

- + Accepts input of variable size, i.e. sequences (time series, sentences etc)
 - Can even be used to process tree-structured inputs by using Tree-LSTMs [Tai et. al., 2015]

- + Accepts input of variable size, i.e. sequences (time series, sentences etc)
 - Can even be used to process tree-structured inputs by using Tree-LSTMs [Tai et. al., 2015]
- + May learn long-term dependencies

- + Accepts input of variable size, i.e. sequences (time series, sentences etc)
 - Can even be used to process tree-structured inputs by using Tree-LSTMs [Tai et. al., 2015]
- + May learn long-term dependencies
- Training may be slow when sequence length is large

At IPRally we work on automated patent searches. The basic idea is the following:

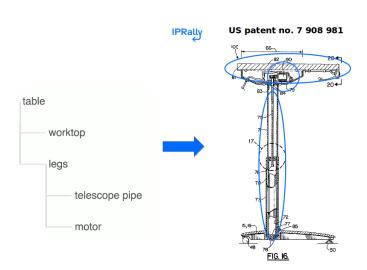
Patents are transformed to graphs by extracting the relevant information from the patent claims and specifications

- Patents are transformed to graphs by extracting the relevant information from the patent claims and specifications
- The graphs are then embedded to vectors by using a Tree-LSTM model

- Patents are transformed to graphs by extracting the relevant information from the patent claims and specifications
- The graphs are then embedded to vectors by using a Tree-LSTM model
 - The model is trained by using millions of real-life positive and negative novelty citations from previous patent applications

- Patents are transformed to graphs by extracting the relevant information from the patent claims and specifications
- The graphs are then embedded to vectors by using a Tree-LSTM model
 - The model is trained by using millions of real-life positive and negative novelty citations from previous patent applications
 - Patents with a positive citation get vectors that are close to each other

- Patents are transformed to graphs by extracting the relevant information from the patent claims and specifications
- The graphs are then embedded to vectors by using a Tree-LSTM model
 - The model is trained by using millions of real-life positive and negative novelty citations from previous patent applications
 - Patents with a positive citation get vectors that are close to each other
- 3 A prior art search for a new patent can then be done by searching for the nearest neighbors of the vector created from the new invention



Convolutional neural network (CNN)

TODO: Picture here Extracts features of two-dimensional input (usually an image) using convolutional and pooling layers.

+ Works well with image data

- + Works well with image data
- + Training can be effectively parallelized

- + Works well with image data
- + Training can be effectively parallelized
- + Pre-existing models can be fine-tuned for specific tasks

- + Works well with image data
- + Training can be effectively parallelized
- + Pre-existing models can be fine-tuned for specific tasks
- Does not take into account position or orientation of the object

 Finding the optimal neural network layout is often time-consuming

- Finding the optimal neural network layout is often time-consuming
- The model may be sensitive to changes in hyperparameters

- Finding the optimal neural network layout is often time-consuming
- The model may be sensitive to changes in hyperparameters
- A model may take several hours or even days to train
 - This makes hyperparameter searches very expensive

- Write unit tests for your model [Roberts, 2017]
 - Check that each layer actually changes weights
 - Make sure that model converges on tiny data set

- Write unit tests for your model [Roberts, 2017]
 - Check that each layer actually changes weights
 - Make sure that model converges on tiny data set
- Stick to well-known architectures when starting out (e.g. LSTM/GRU for sequential data)

- Write unit tests for your model [Roberts, 2017]
 - Check that each layer actually changes weights
 - Make sure that model converges on tiny data set
- Stick to well-known architectures when starting out (e.g. LSTM/GRU for sequential data)
- Start by using small batch size
 - Usually makes model less sensitive to other hyperparameters

- Write unit tests for your model [Roberts, 2017]
 - Check that each layer actually changes weights
 - Make sure that model converges on tiny data set
- Stick to well-known architectures when starting out (e.g. LSTM/GRU for sequential data)
- Start by using small batch size
 - Usually makes model less sensitive to other hyperparameters
- Use normalization (batch, layer, group, weight...)
 - Speeds up convergence significantly
 - Start by trying batch normalization for CNN and feed-forward nets and layer normalization for RNN

The curious case of the batch size

References

- Nielsen, Michael A. Neural Networks And Deep Learning. Determination Press, 2015. http://neuralnetworksanddeeplearning.com/
- Hornik, Kurt. Approximation Capabilities of Multilayer Feedforward Networks. Neural Networks, 4(2), 251–257, 1991.
- Roberts, Chase. How to unit test machine learning code.

 Medium.com 2017. https://medium.com/@keeper6928/
 how-to-unit-test-machine-learning-code-57cf6fd81765.
- Tai, Kai Sheng et al. Improved Semantic Representations From Tree-Structured Long Short-Term Memory Networks. ACL 2015. https://arxiv.org/abs/1503.00075