Neural networks

Architectures and training tips

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IPRally Technologies

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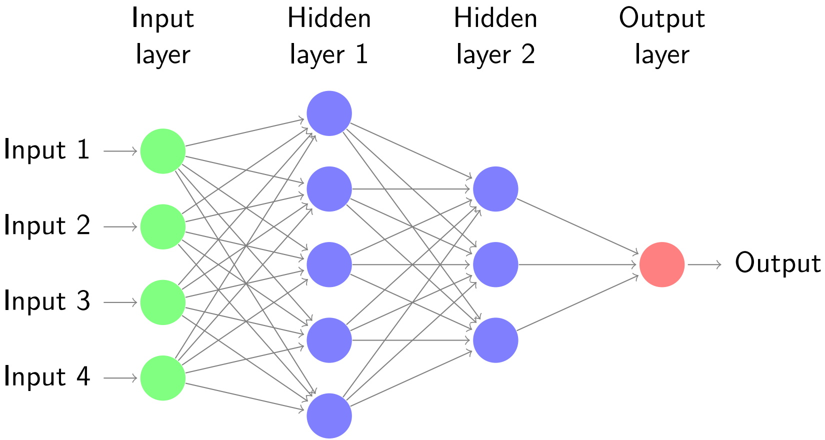
What is a neural network?



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

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

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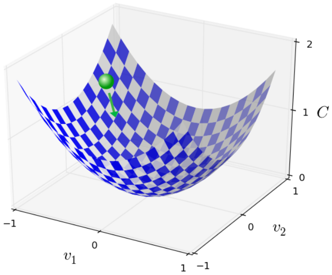
The function f is called the activation function. It must be non-linear to allow the network to learn non-linear dependencies.

Training neural networks using SGD



[Nielsen, 2015], Chapter 1.

The training data is processed in small batches, and the weights of the model are iteratively updated by going in the direction of the negative gradient of the loss function.

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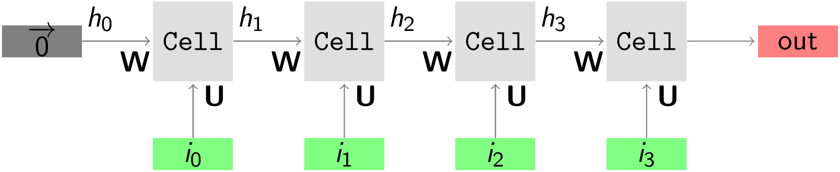
- May learn to respond to unexpected patterns
- Useful especially when the amount of data is large compared to input dimensionality
- Less need for feature engineering compared to traditional ML methods

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:

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

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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.

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- Prediction accuracy may also suffer if the sequence is long
  - The model may not remember early inputs and can be biased toward the end of the sequence

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2. 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

RNN real life use case: Patent search

- table
  - worktop
  - legs
    - telescope pipe
    - motor

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US patent no. 7 908 981

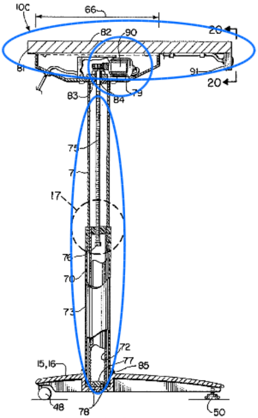

FIG. 16.

Convolutional neural network (CNN)

Feed-forward networks do not scale well to images due to the large input size. Convolutional neural networks are constrained to looking only at a small part of the image at a time, and thus the number of weights stays manageable.

A CNN uses three types of layers: convolutional, pooling and fully connected.

CNN - Convolutional layer

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- Each individual filter is small (i.e. small height and width)
- During the forward pass we slide each filter across the entire input and compute dot products between input entries and filter weights
- The idea is that each filter learns to identify some kind of feature (for instance part of a shape)

CNN - Convolutional layer

0	0	0	0	0
0	1	1	1	0
0	1	0	1	0
0	1	1	1	0
0	0	0	0	0

CNN - Convolutional layer

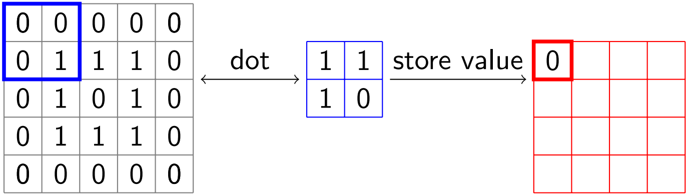
0	0	0	0	0
0	1	1	1	0
0	1	0	1	0
0	1	1	1	0
0	0	0	0	0

1	1
1	0

CNN - Convolutional layer

$$
\begin{array}{|c|c|c|c|c|}
\hline
0 & 0 & 0 & 0 & 0 \\ \hline
0 & 1 & 1 & 1 & 0 \\ \hline
0 & 1 & 0 & 1 & 0 \\ \hline
0 & 1 & 1 & 1 & 0 \\ \hline
0 & 0 & 0 & 0 & 0 \\ \hline
\end{array}
\quad \xleftrightarrow{\text{dot}} \quad
\begin{array}{|c|c|}
\hline
1 & 1 \\ \hline
1 & 0 \\ \hline
\end{array}
\qquad\qquad
\begin{array}{|c|c|c|c|}
\hline
 & & & \\ \hline
 & & & \\ \hline
 & & & \\ \hline
 & & & \\ \hline
\end{array}
$$

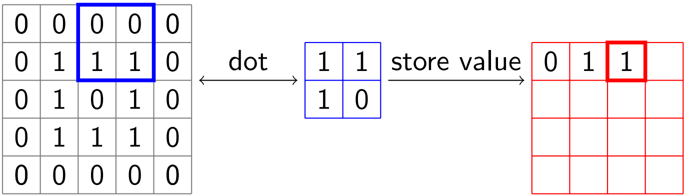
CNN - Convolutional layer



CNN - Convolutional layer

$$\begin{array}{|c|c|c|c|c|}\hline 0 & 0 & 0 & 0 & 0 \\ \hline 0 & 1 & 1 & 1 & 0 \\ \hline 0 & 1 & 0 & 1 & 0 \\ \hline 0 & 1 & 1 & 1 & 0 \\ \hline 0 & 0 & 0 & 0 & 0 \\ \hline \end{array} \xleftrightarrow{\text{dot}} \begin{array}{|c|c|}\hline 1 & 1 \\ \hline 1 & 0 \\ \hline \end{array} \xrightarrow{\text{store value}} \begin{array}{|c|c|c|c|}\hline 0 & \boxed{1} & & \\ \hline & & & \\ \hline & & & \\ \hline & & & \\ \hline \end{array}$$

CNN - Convolutional layer



CNN - Convolutional layer

$$
\begin{array}{|c|c|c|c|c|}
\hline
0 & 0 & 0 & 0 & 0 \\ \hline
0 & 1 & 1 & 1 & 0 \\ \hline
0 & 1 & 0 & 1 & 0 \\ \hline
0 & 1 & 1 & 1 & 0 \\ \hline
0 & 0 & 0 & 0 & 0 \\ \hline
\end{array}
\xleftrightarrow{\text{dot}}
\begin{array}{|c|c|}
\hline
1 & 1 \\ \hline
1 & 0 \\ \hline
\end{array}
\xrightarrow{\text{store value}}
\begin{array}{|c|c|c|c|}
\hline
0 & 1 & 1 & \boxed{1} \\ \hline
 & & & \\ \hline
 & & & \\ \hline
 & & & \\ \hline
\end{array}
$$

CNN - Convolutional layer

$$\begin{array}{|c|c|c|c|c|}\hline 0 & 0 & 0 & 0 & 0 \\ \hline 0 & 1 & 1 & 1 & 0 \\ \hline 0 & 1 & 0 & 1 & 0 \\ \hline 0 & 1 & 1 & 1 & 0 \\ \hline 0 & 0 & 0 & 0 & 0 \\ \hline \end{array} \xleftrightarrow{\text{dot}} \begin{array}{|c|c|}\hline 1 & 1 \\ \hline 1 & 0 \\ \hline \end{array} \xrightarrow{\text{store value}} \begin{array}{|c|c|c|c|}\hline 0 & 1 & 1 & 1 \\ \hline \boxed{1} & & & \\ \hline & & & \\ \hline & & & \\ \hline \end{array}$$

CNN - Convolutional layer

$$\begin{array}{|c|c|c|c|c|}\hline 0&0&0&0&0\\\hline 0&1&1&1&0\\\hline 0&1&0&1&0\\\hline 0&1&1&1&0\\\hline 0&0&0&0&0\\\hline\end{array} \xleftrightarrow{\text{dot}} \begin{array}{|c|c|}\hline 1&1\\\hline 1&0\\\hline\end{array} \xrightarrow{\text{store value}} \begin{array}{|c|c|c|c|}\hline 0&1&1&1\\\hline 1&\boxed{3}&&\\\hline &&&\\\hline &&&\\\hline\end{array}$$

CNN - Convolutional layer

$$\begin{bmatrix}0&0&0&0&0\\0&1&1&1&0\\0&1&0&1&0\\0&1&1&1&0\\0&0&0&0&0\end{bmatrix} \xleftrightarrow{\text{dot}} \begin{bmatrix}1&1\\1&0\end{bmatrix} \xrightarrow{\text{store value}} \begin{bmatrix}0&1&1&1\\1&3&\boxed{2}&\\&&&\\&&&\end{bmatrix}$$

CNN - Convolutional layer

$$
\begin{array}{|c|c|c|c|c|}
\hline
0 & 0 & 0 & 0 & 0 \\
\hline
0 & 1 & 1 & 1 & 0 \\
\hline
0 & 1 & 0 & 1 & 0 \\
\hline
0 & 1 & 1 & 1 & 0 \\
\hline
0 & 0 & 0 & 0 & 0 \\
\hline
\end{array}
\xleftrightarrow{\text{dot}}
\begin{array}{|c|c|}
\hline
1 & 1 \\
\hline
1 & 0 \\
\hline
\end{array}
\xrightarrow{\text{store value}}
\begin{array}{|c|c|c|c|}
\hline
0 & 1 & 1 & 1 \\
\hline
1 & 3 & 2 & \boxed{2} \\
\hline
 & & & \\
\hline
 & & & \\
\hline
\end{array}
$$

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$$\begin{array}{|c|c|c|c|c|}\hline 0&0&0&0&0\\ \hline 0&1&1&1&0\\ \hline 0&1&0&1&0\\ \hline 0&1&1&1&0\\ \hline 0&0&0&0&0\\ \hline \end{array} \xleftrightarrow{\text{dot}} \begin{array}{|c|c|}\hline 1&1\\ \hline 1&0\\ \hline \end{array} \xrightarrow{\text{store value}} \begin{array}{|c|c|c|c|}\hline 0&1&1&1\\ \hline 1&3&2&2\\ \hline \boxed{1}& & & \\ \hline & & & \\ \hline \end{array}$$

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$$\begin{array}{|c|c|c|c|c|}\hline 0&0&0&0&0\\\hline 0&1&1&1&0\\\hline 0&1&0&1&0\\\hline 0&1&1&1&0\\\hline 0&0&0&0&0\\\hline\end{array} \xleftrightarrow{\text{dot}} \begin{array}{|c|c|}\hline 1&1\\\hline 1&0\\\hline\end{array} \xrightarrow{\text{store value}} \begin{array}{|c|c|c|c|}\hline 0&1&1&1\\\hline 1&3&2&2\\\hline 1&2&\boxed{2}&\\\hline &&&\\\hline\end{array}$$

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\begin{array}{|c|c|c|c|c|}
\hline
0 & 0 & 0 & 0 & 0 \\
\hline
0 & 1 & 1 & 1 & 0 \\
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\hline
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\hline
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\hline
1 & 1 \\
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\hline
\end{array}
\xrightarrow{\text{store value}}
\begin{array}{|c|c|c|c|}
\hline
0 & 1 & 1 & 1 \\
\hline
1 & 3 & 2 & 2 \\
\hline
1 & 2 & 2 & \boxed{2} \\
\hline
 & & & \\
\hline
\end{array}
$$

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$$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix} \xleftrightarrow{\text{dot}} \begin{bmatrix} 1 & 1 \\ 1 & 0 \end{bmatrix} \xrightarrow{\text{store value}} \begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 3 & 2 & 2 \\ 1 & 2 & 2 & 2 \\ 1 & & & \end{bmatrix}$$

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0	0	0	0	0
0	1	1	1	0
0	1	0	1	0
0	1	1	1	0
0	0	0	0	0

$\xleftrightarrow{\text{dot}}$

1	1
1	0

$\xrightarrow{\text{store value}}$

0	1	1	1
1	3	2	2
1	2	2	2
1	2		

CNN - Convolutional layer

$$\begin{array}{|c|c|c|c|c|}\hline 0 & 0 & 0 & 0 & 0 \\ \hline 0 & 1 & 1 & 1 & 0 \\ \hline 0 & 1 & 0 & 1 & 0 \\ \hline 0 & 1 & 1 & 1 & 0 \\ \hline 0 & 0 & 0 & 0 & 0 \\ \hline \end{array} \xleftrightarrow{\text{dot}} \begin{array}{|c|c|}\hline 1 & 1 \\ \hline 1 & 0 \\ \hline \end{array} \xrightarrow{\text{store value}} \begin{array}{|c|c|c|c|}\hline 0 & 1 & 1 & 1 \\ \hline 1 & 3 & 2 & 2 \\ \hline 1 & 2 & 2 & 2 \\ \hline 1 & 2 & \boxed{2} & \\ \hline \end{array}$$

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- A common way is to take the maximum value of a small grid (max pooling)
  - For instance if we use max pooling with a filter of size 2x2 we discard 75 percent of the values

CNN - Pooling layer

0	1	1	1
1	3	2	2
1	2	2	2
1	2	2	1

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0	1	1	1
1	3	2	2
1	2	2	2
1	2	2	1

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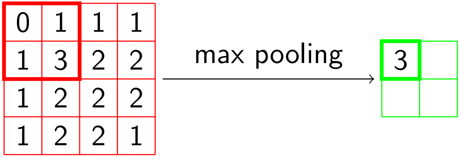

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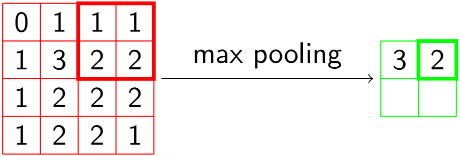

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$$\begin{array}{|c|c|c|c|}\hline 0 & 1 & 1 & 1 \\ \hline 1 & 3 & 2 & 2 \\ \hline 1 & 2 & 2 & 2 \\ \hline 1 & 2 & 2 & 1 \\ \hline \end{array} \xrightarrow{\text{max pooling}} \begin{array}{|c|c|}\hline 3 & 2 \\ \hline \boxed{2} & \\ \hline \end{array}$$

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$$
\begin{array}{|c|c|c|c|}
\hline
0 & 1 & 1 & 1 \\
\hline
1 & 3 & 2 & 2 \\
\hline
1 & 2 & 2 & 2 \\
\hline
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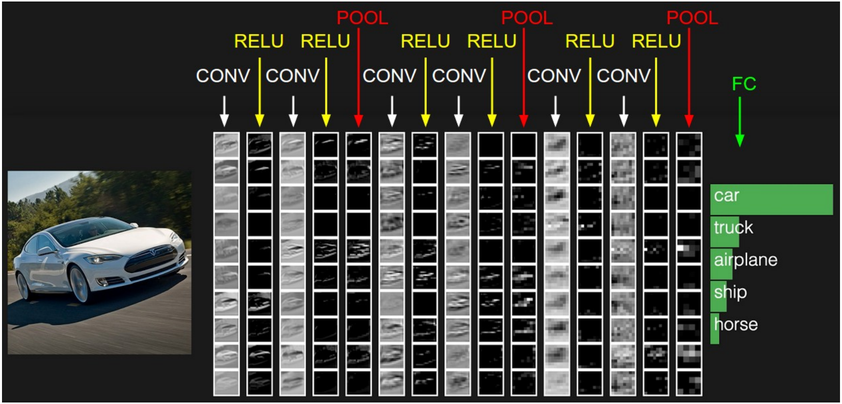
\hline
\end{array}
\xrightarrow{\text{max pooling}}
\begin{array}{|c|c|}
\hline
3 & 2 \\
\hline
2 & \boxed{2} \\
\hline
\end{array}
$$

CNN - Example architecture



Taken from http://cs231n.github.io/convolutional-networks/

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− Does not take into account orientation of the object

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- The model may be sensitive to changes in hyperparameters, especially learning rate and activation function
- A model may take several hours or even days to train
  - This makes hyperparameter searches very expensive
- It's often hard to know why the model predicts as it does because of the complexity of the model

Tips and tricks

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  - Check that each layer actually changes weights
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- 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
  - See [Kurita, 2018] for a good overview

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- Training of neural nets can be sped up by increasing the batch size, since then the GPU/TPU can process more training examples in parallel.
- Increasing the batch size decreases the variance of the gradient estimates, but only by the square root of the increase.
- In practice increasing the batch size may result in a worse model. In extreme cases the model might not learn anything at all! [Masters et. al., 2018]

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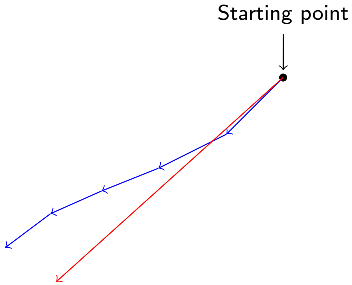
    - Otherwise the magnitude of the weight updates decreases
- This means that increasing the batch size trades computational efficiency for stale gradients
- Training with large batches often converge to sharp minimizers, and this leads to worse test performance [Keskar et. al., 2016]

The curious case of the batch size



- Blue arrows - gradient updates with small batch size
- Red arrow - gradient updates with large batch size
- There is no guarantee that taking a larger step using the gradient in the original step leads to the same result as taking several smaller steps.

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  - Another solution is to use a small batch size in the beginning and increase it when the speed of the model change decreases

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