

# 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/>

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

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

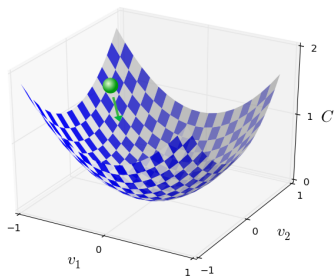
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The function  $f$  is called the activation function. It must be non-linear to allow the network to learn non-linear dependencies.

# 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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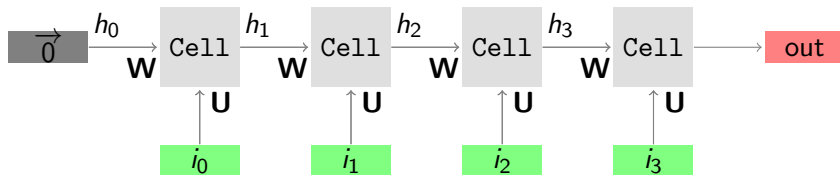
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# Why neural networks?

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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.

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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:

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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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  - 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

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US patent no. 7 908 981

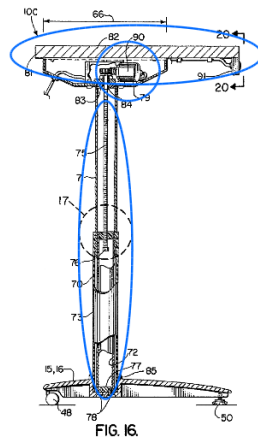
table

worktop

legs

telescope pipe

motor



# 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.

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- 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

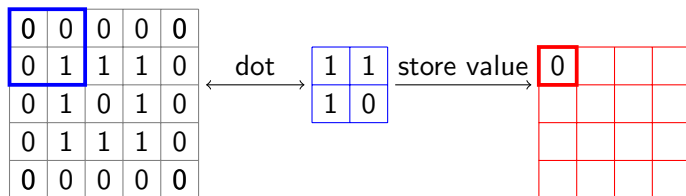
0	0	0	0	0
0	1	1	1	0
0	1	0	1	0
0	1	1	1	0
0	0	0	0	0

dot

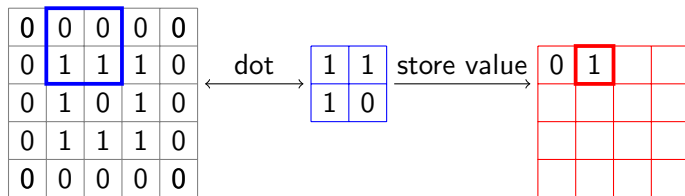


1	1
1	0

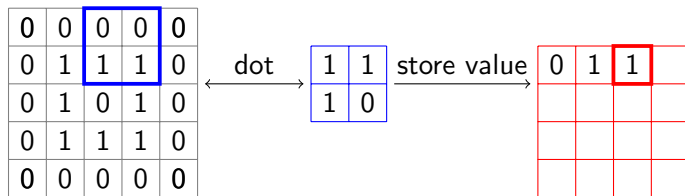

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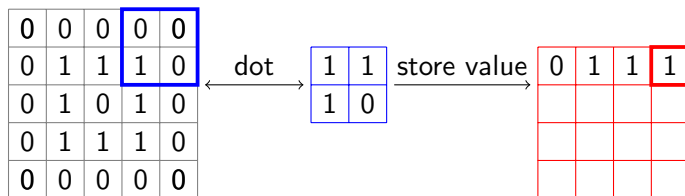
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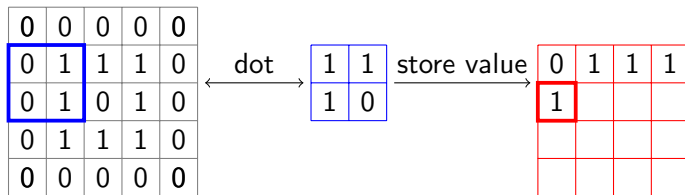


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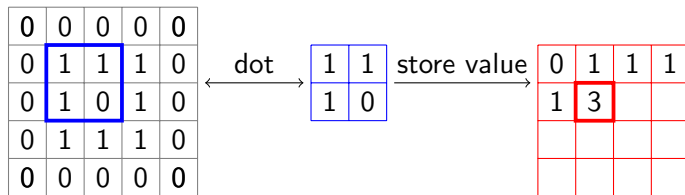




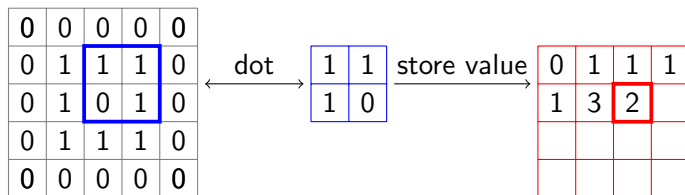
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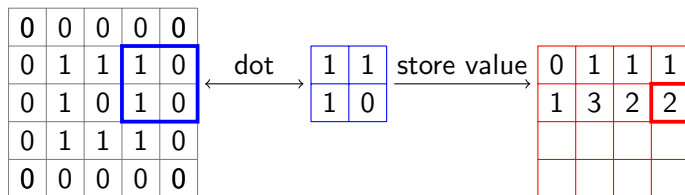
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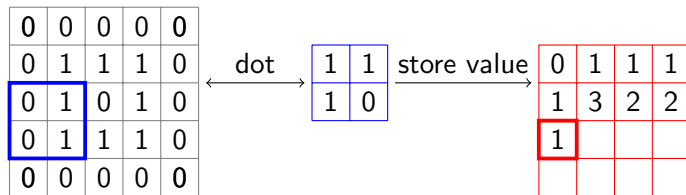
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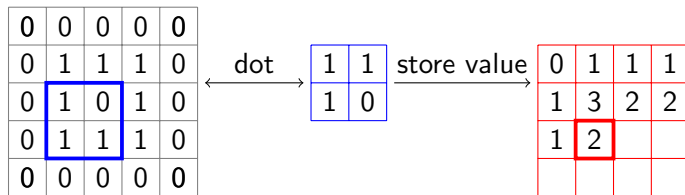
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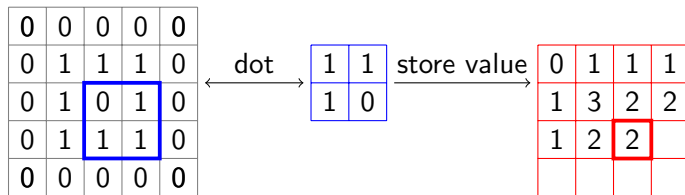
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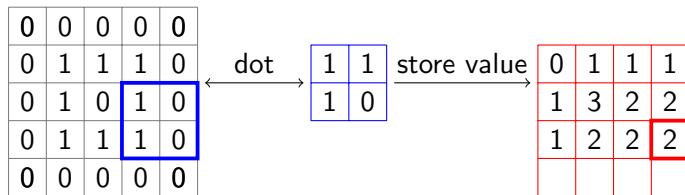
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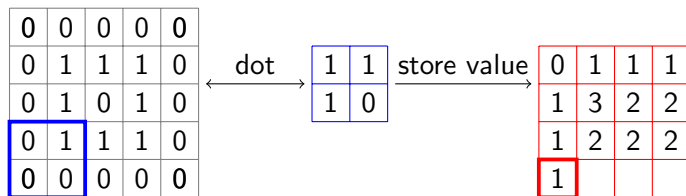


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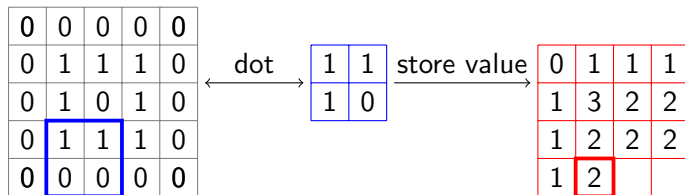




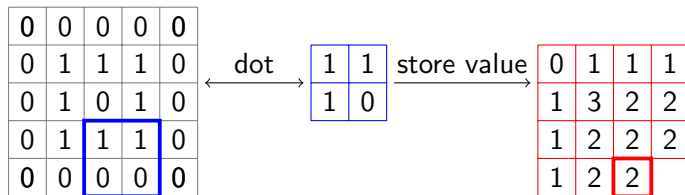
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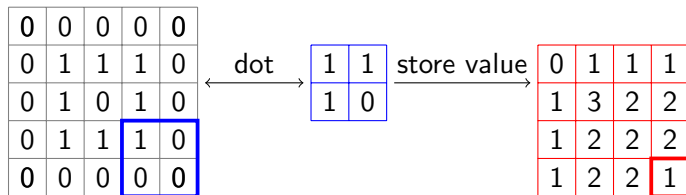
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  - This is done to decrease the amount of computation in the network
- A common way is to take the maximum value of a small grid (max pooling)
  - For instance if we use max pooling with a filter of size  $2 \times 2$  we discard 75 percent of the values

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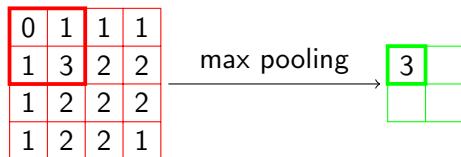
0	1	1	1
1	3	2	2
1	2	2	2
1	2	2	1

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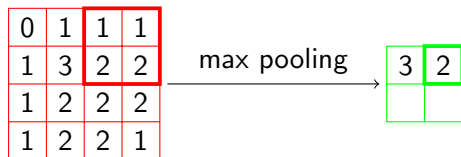
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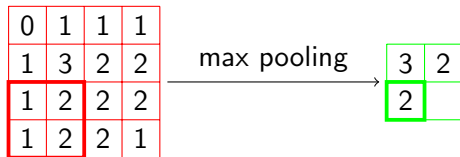
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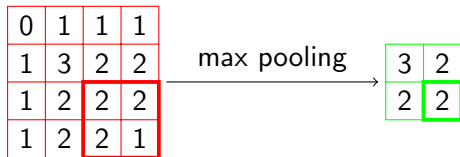
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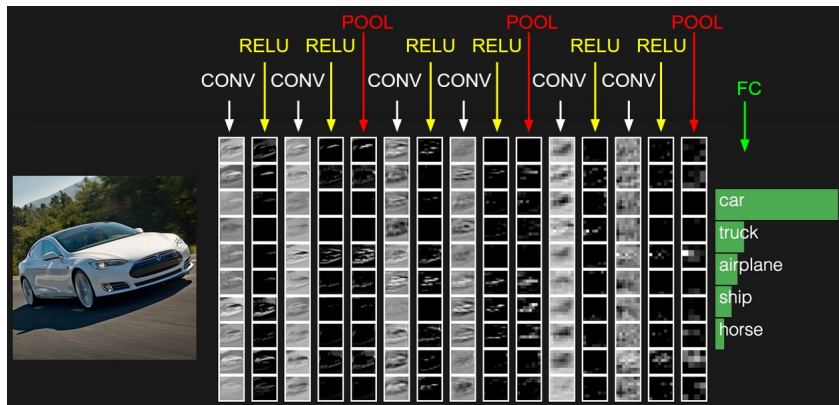
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# CNN - Example architecture



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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  - 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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- Start by using small batch size (for instance 32)
  - 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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  - Note that the learning rates that work are affected by the chosen batch size
- A good optimizer to try out first is Adam (with default parameters other than learning rate)

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- Increasing the batch size decreases the standard deviation 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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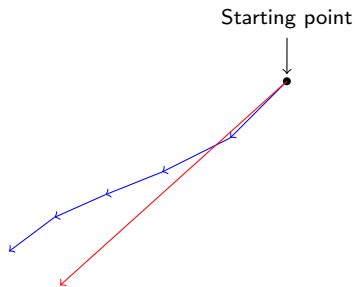
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- Training with large batches often converge to sharp minimizers, and this leads to worse test performance [Keskar et. al., 2016]
  - The randomness of the small batch size may actually help to find better local minima!

# 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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  - A smaller learning rate was used early to avoid optimization challenges early in the training
  - Another solution is to use a small batch size in the beginning and increase it when the speed of the model change decreases

# References I



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>.



Kurita, Keita. *An Overview of Normalization Methods in Deep Learning*. <http://mlexplained.com/2018/11/30/an-overview-of-normalization-methods-in-deep-learning/>.

# References II

-  Tai, Kai Sheng et al. *Improved Semantic Representations From Tree-Structured Long Short-Term Memory Networks*. *ACL 2015*. <https://arxiv.org/abs/1503.00075>
-  Masters, Dominic, Luschi, Carlo. Revisiting Small Batch Training for Deep Neural Networks. arXiv preprint 2018. <https://arxiv.org/abs/1804.07612>
-  Keskar Nitish, et. al. *On Large-Batch Training for Deep Learning: Generalization Gap and Sharp Minima*. *ICLR 2017 conference paper* <https://arxiv.org/abs/1609.04836>
-  Goyal, Priya et. al. Accurate, Large Minibatch SGD: Training ImageNet in 1 Hour arXiv preprint 2017. <https://arxiv.org/abs/1706.02677>