Deep Learning

Texts in Computer Science

Michael R. Berthold · Christian Borgelt Frank Höppner · Frank Klawonn Rosaria Silipo

Guide to Intelligent Data Science

How to Intelligently Make Use of Real Data

Second Edition



Summary of this lesson

"What people call AI is no more than finding answers to questions we know to ask. Real AI is answering questions we haven't dreamed of yet"

-Tom Golway

How deep can we dig in AI?

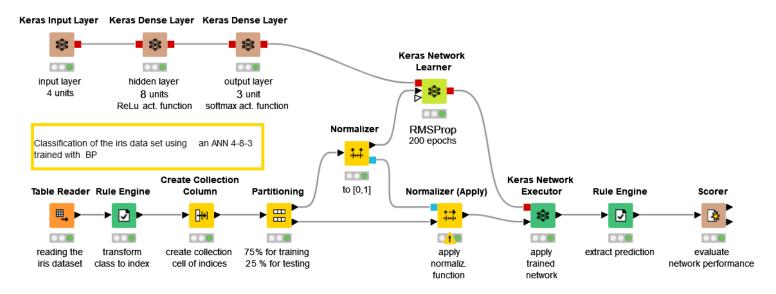
*This lesson refers to chapter 9 of the GIDS book

Content of this Lesson

- Recurrent Neiral Networks (RNNs)
- Long Short Term Memories (LSTMs)
- Convolutional Neural networks (CNNs)
- Generative Adversarial Networks (GANs)

Datasets

- Datasets used : iris dataset
- Example Workflows:
 - "Classifying the iris data set with ANN" https://kni.me/w/ei3eX9Sj5-RFEUat
 - Keras layers
 - Multi-layer perceptrion
 - Back propagation



Deep Learning

- Deep Learning is the recent evolution of Neural Networks
- It covers:
 - Feedforward networks with many hidden layers (deep ©)
 - New paradigms, like LSTMs in Recurrent Neural Networks, suitable for time series analysis
 - New topological layers, like convolutional and pooling layers, mainly for image processing
 - New architectures as in Generative Adversarial Networks (GANs)
 - ...
- Improvements are mainly due to:
 - Increased computational power for faster calculations, like GPUs
 - Parallel Computation

Recurrent Neural Networks (RNNs)

What are Recurrent Neural Networks?

- Recurrent Neural Networks (RNNs) are a family of neural networks suitable for processing of sequential data
- RNNs include auto and backward connections

- RNNs are used for all sorts of tasks:
 - Language modeling / Text generation
 - Text classification
 - Neural machine translation
 - Image captioning
 - Speech to text
 - Numerical time series data, e.g. sensor data
 - Time series analysis

- ...

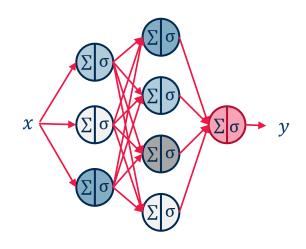
Why do we need RNNs for Sequential Data?

Goal: Translation from German to English

 Option One: Use feed forward network to translate word by word

But what happens with this question?

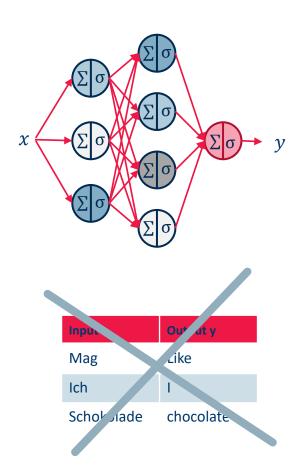
"Mag ich Schokolade?" => "Do I like chocolate?"



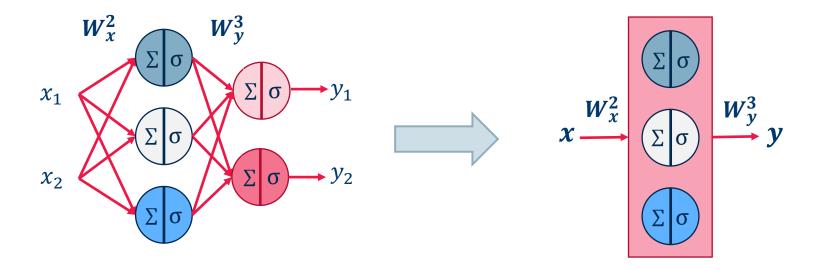
Input x	Output y
Ich	I
mag	like
Schokolade	chocolate

Why do we need RNNs for Sequential Data?

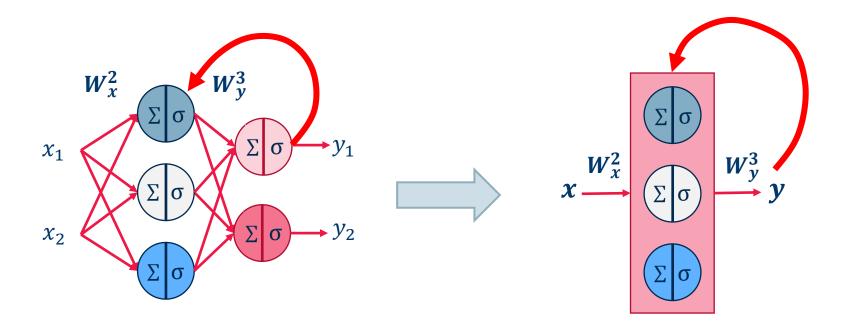
- Problems with FFNN:
 - Each time step is completely independent
 - For translations we need context
 - More general: we need a network that remembers inputs from the past
- Solution: Recurrent Neural Networks



From Feed Forward to Recurrent Neural Networks

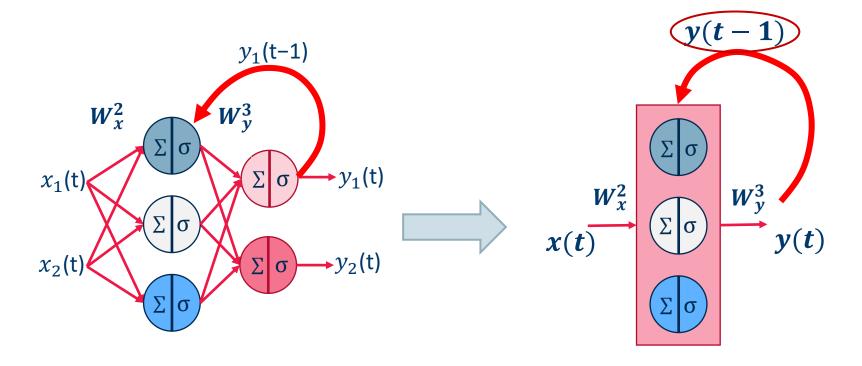


From Feed Forward to Recurrent Neural Networks



- A Recurrent Neural Network is a FFNN with auto and/or backward connections
- Recurrent connections introduce the concept of time in FFNNs

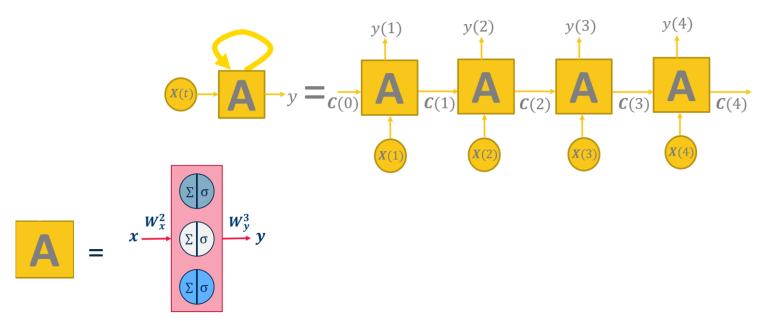
From Feed Forward to Recurrent Neural Networks



- A Recurrent Neural Network is a FFNN with auto and/or backward connections
- Recurrent connections introduce the concept of time in FFNNs

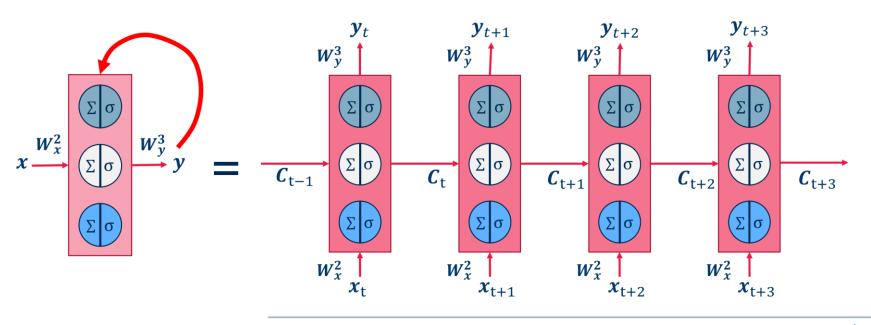
How can we represent a RNN over time?

- At every time t, FFNN A has two inputs:
 - **x**(t)
 - some shape of y(t-1) -> state of network A: C(t-1)
- The recurrent network can then be unrolled over time around A



Unrolling of a RNN over time

The unrolled version of the original network in *m* intermediate steps becomes a FFNN and can be trained with BackPropagation: **Back-Propagation Through Time (BPTT).**



time t

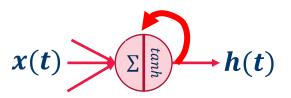
Summarizing: RNNs and BPTT

- Neural network architectures with recurring connections on some units are named Recurrent Neural Networks (RNNs).
- Adding a recurrent connection to one unit might store information about past inputs in the evolving status of the unit.
- Training set: {**X**(t), y(t) } for t=1, 2, ... N.
- For each X(t), the recurrent connection requires m steps into the future to produce the final output.
- An easy trick to represent the recurrent network is to unroll it into m copies of the feedforward internal block "A", each with their set of static weight matrix W. Each copy of "A" receives inputs X(t) and C(t-1) and produces output y(t).
- A modified version of the Back-Propagation algorithm is used to train the unrolled version in *m* intermediate steps of the original neural architecture: Back-Propagation Through Time (BPTT).

Long Short Term Memory

Simple Recurrent Unit

The simplest possible recurrent unit is a neuron with an auto-connection.



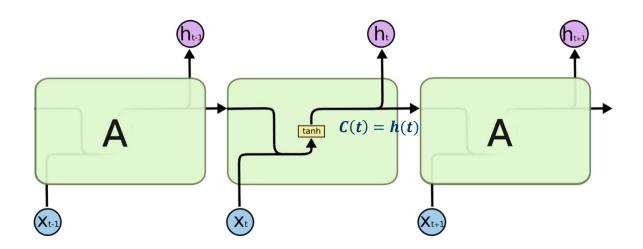


Image Source: Christopher Olah, https://colah.github.io/posts/2015-08-Understanding-LSTMs/

Limitations of Layers with Simple Recurrent Units

The "memory" of simple RNNs is sometimes too limited to be useful:

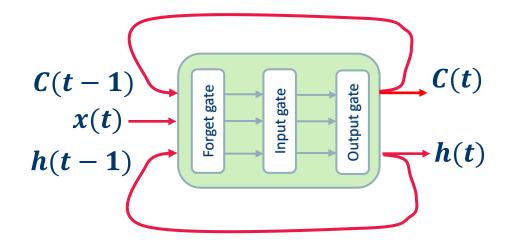
- "Cars drive on the ____" (road)
- "I love the beach.My favorite sound is the crashing of the _____" (cars? glass? waves?)

Sometimes we need to go back deeper in time

LSTM = Long Short Term Memory

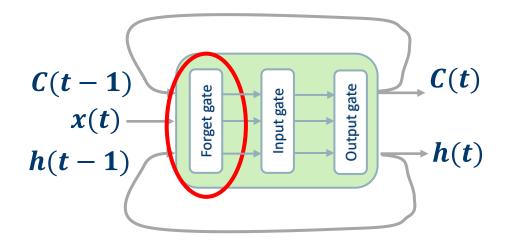
This is an engineered type of unit with three gates:

- Forget gate
- Input gate
- Output gate

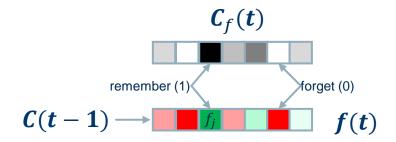


This is an engineered type of unit with three gates:

- Forget gate
- Input gate
- Output gate

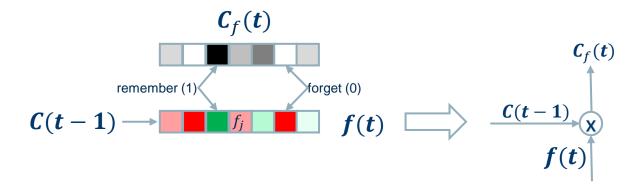


- Forget Gate is trained to forget the status.
- At time t, the forget gate decides which item of C(t-1) to keep (and how much of it) in C(t), given input vector x(t) and previous output h(t-1).



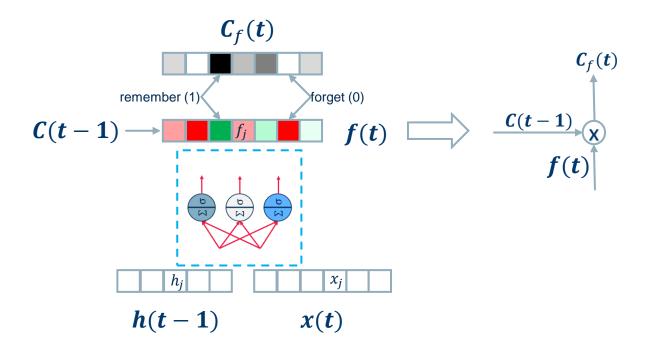


- Forget Gate is trained to forget the status.
- At time t, the forget gate decides which item of C(t-1) to keep (and how much of it) in C(t), given input vector x(t) and previous output h(t-1).

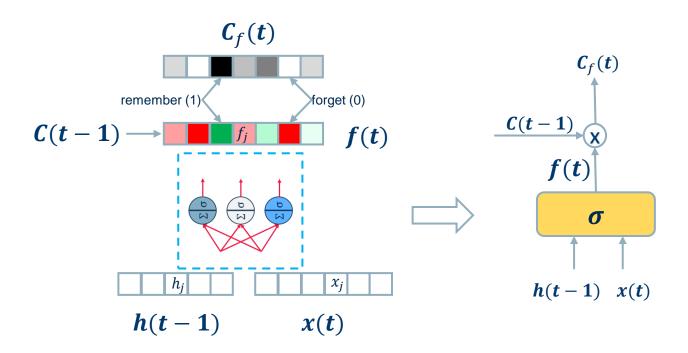




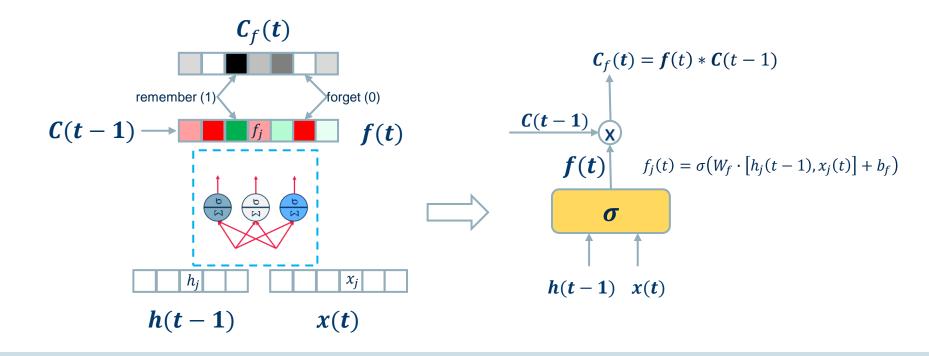
- Forget Gate is trained to forget the status.
- At time t, the forget gate decides which item of C(t-1) to keep (and how much of it) in C(t), given input vector x(t) and previous output h(t-1).



- Forget Gate is trained to forget the status.
- At time t, the forget gate decides which item of C(t-1) to keep (and how much of it) in C(t), given input vector x(t) and previous output h(t-1).

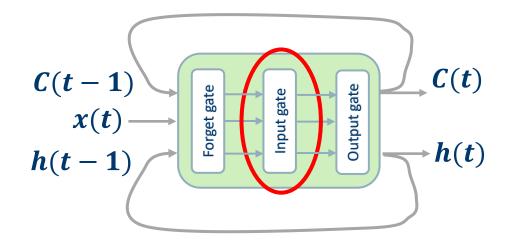


- Forget Gate is trained to forget the status.
- At time t, the forget gate decides which item of C(t-1) to keep (and how much of it) in C(t), given input vector x(t) and previous output h(t-1).



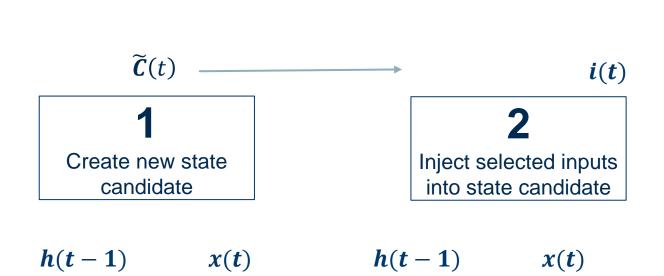
This is an engineered type of unit with three gates:

- Forget gate
- Input gate
- Output gate



- Input Gate is trained to inject significant parts of the current input into the status.
- At time t, the input gate decides which item of x(t) to inject (and how much of it) into C(t), given input vector x(t) and previous output h(t-1).

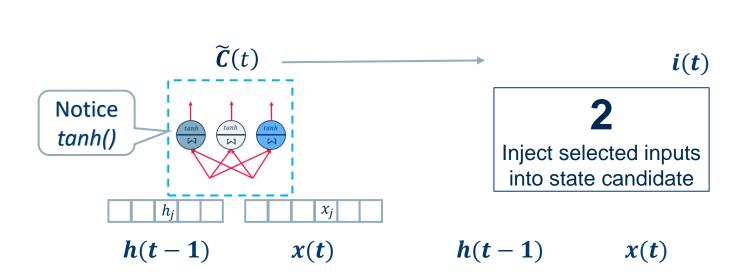
 $C_i(t)$



LSTM: Input Gate – create new state candidate

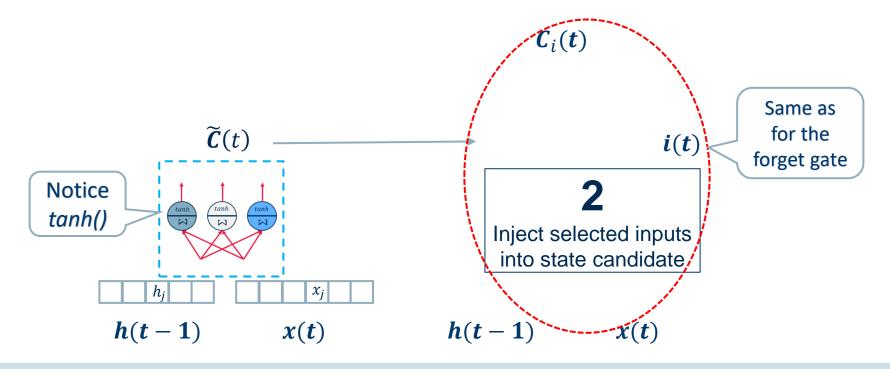
- Input Gate is trained to inject significant parts of the current input into the status.
- At time t, the input gate decides which item of x(t) to inject (and how much of it) into C(t), given input vector x(t) and previous output h(t-1).

 $C_i(t)$



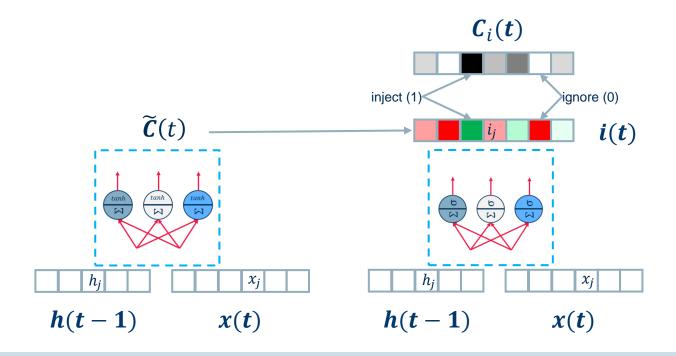
LSTM: Input Gate – inject input

- Input Gate is trained to inject significant parts of the current input into the status.
- At time t, the input gate decides which item of x(t) to inject (and how much of it) into C(t), given input vector x(t) and previous output h(t-1).

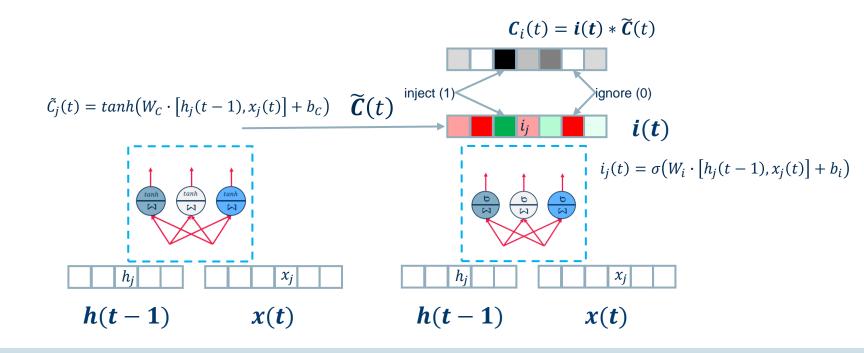


LSTM: Input Gate – inject input

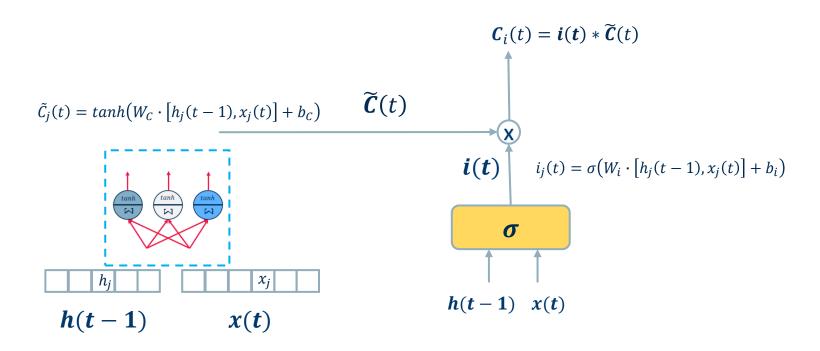
- Input Gate is trained to inject significant parts of the current input into the status.
- At time t, the input gate decides which item of x(t) to inject (and how much of it) into C(t), given input vector x(t) and previous output h(t-1).



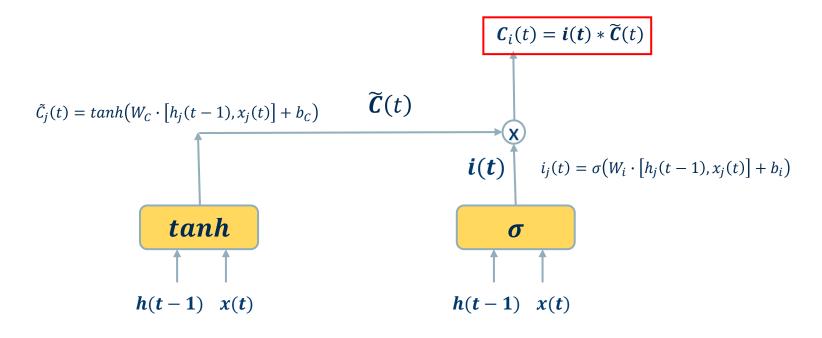
- Input Gate is trained to inject significant parts of the current input into the status.
- At time t, the input gate decides which item of x(t) to inject (and how much of it) into C(t), given input vector x(t) and previous output h(t-1).



- Input Gate is trained to inject significant parts of the current input into the status.
- At time t, the input gate decides which item of x(t) to inject (and how much of it) into C(t), given input vector x(t) and previous output h(t-1).

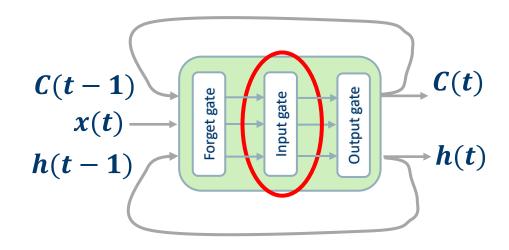


- Input Gate is trained to inject significant parts of the current input into the status.
- At time t, the input gate decides which item of x(t) to inject (and how much of it) into C(t), given input vector x(t) and previous output h(t-1).



This is an engineered type of unit with three gates:

- Forget gate
- Input gate
- Output gate

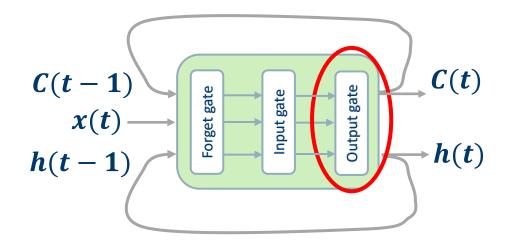


$$\boldsymbol{C}(t) = \boldsymbol{C}_f(t) + \boldsymbol{C}_i(t) = \boldsymbol{f}(t) * \boldsymbol{C}(t-1) + \boldsymbol{i}(t) * \widetilde{\boldsymbol{C}}(t)$$

LSTM = Output Gate

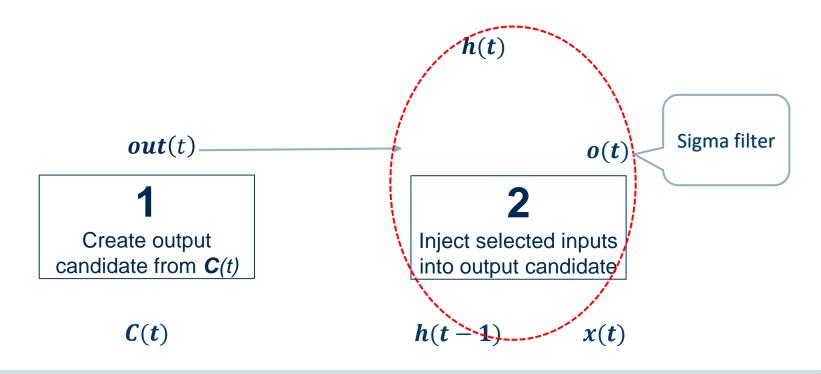
This is an engineered type of unit with three gates:

- Forget gate
- Input gate
- Output gate



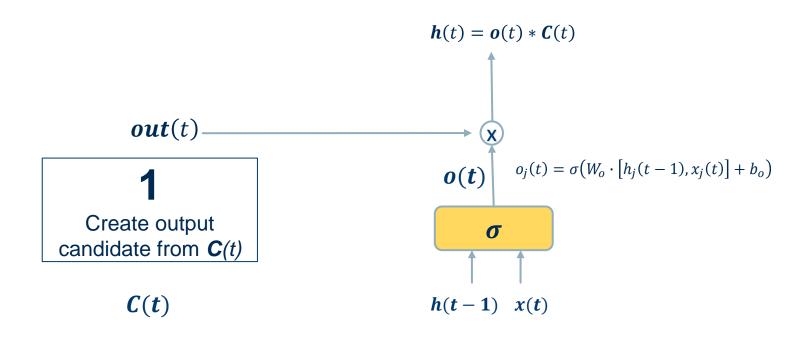
LSTM: Output Gate – input inject into status

- Output Gate is trained to output a reasonable result.
- At time t, output gate decides which parts of status C(t) (and how much of it) will be output, given input vector x(t) and previous output h(t-1).



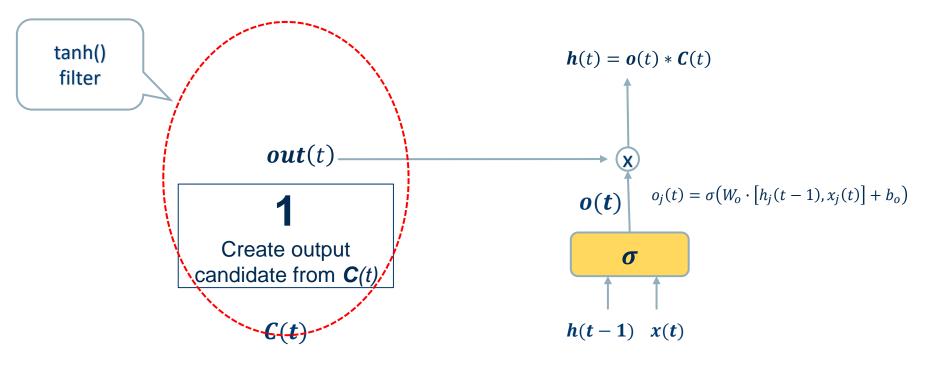
LSTM: Input Gate – input inject into status

- Output Gate is trained to output a reasonable result.
- At time t, output gate decides which parts of status C(t) (and how much of it) will be output, given input vector x(t) and previous output h(t-1).



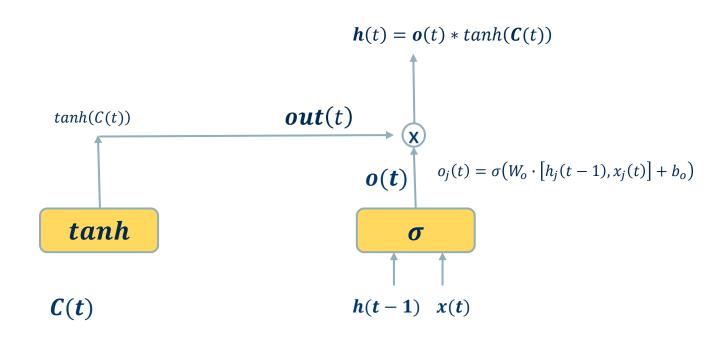
LSTM: Input Gate – prepare output candidate

- Output Gate is trained to output a reasonable result.
- At time t, output gate decides which parts of status C(t) (and how much of it) will be output, given input vector x(t) and previous output h(t-1).



LSTM: Input Gate – prepare output candidate

- Output Gate is trained to output a reasonable result.
- At time t, output gate decides which parts of status C(t) (and how much of it) will be output, given input vector x(t) and previous output h(t-1).



LSTM = Long Short Term Memory

Special type of unit with three gates

Forget gate Input gate Output gate

- Forget gate
- Input gate

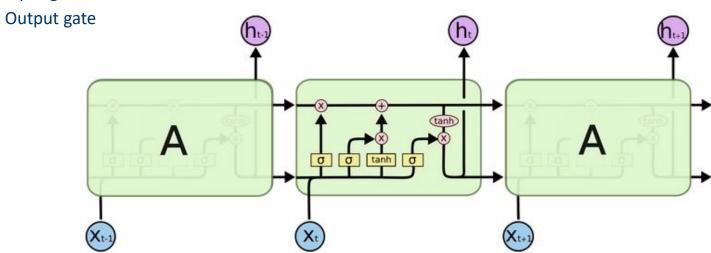
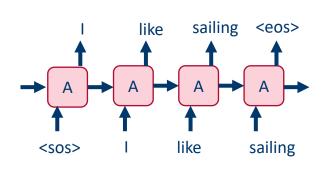


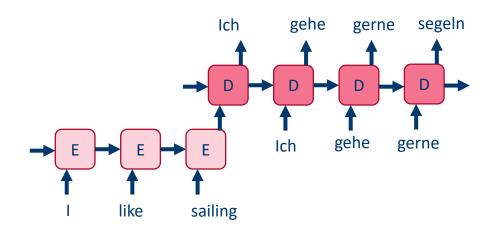
Image Source: Christopher Olah, https://colah.github.io/posts/2015-08-Understanding-LSTMs/

Different Network-Structures and Applications

Many to Many



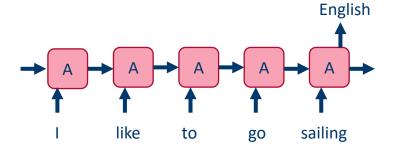
Language model



Neural machine translation

Different Network-Structures and Applications

Many to one



Language classification
Text classification

One to many

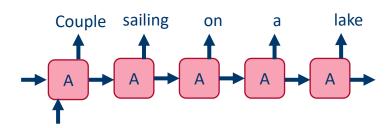
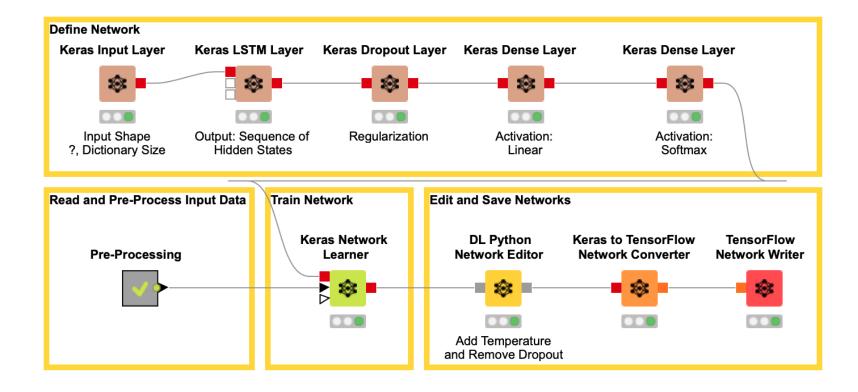




Image captioning

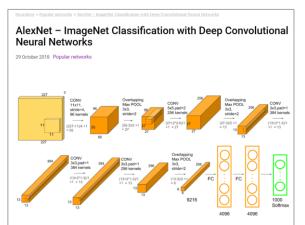
Neural Network: Code-free Example



Convolutional Neural Networks (CNNs)

AlexNet & friends

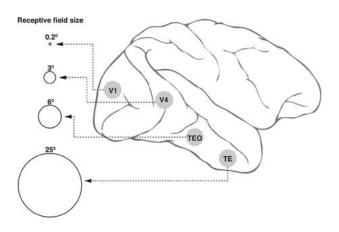
- The big breakthrough in deep learning happened in 2012 with deep convolutional neural networks
- Here deep learning based AlexNet network won the ImageNet challenge with an unprecedented margin.
- The top-five error rate of AlexNet was 15 percent, while the next best competitor ended up with 26 percent.
- This victory kicked off the surge in deep learning networks.



https://neurohive.io/en/popular-networks/alexnet-imagenet-classification-with-deep-convolutional-neural-networks/

Convolutional Neural Networks - CNN

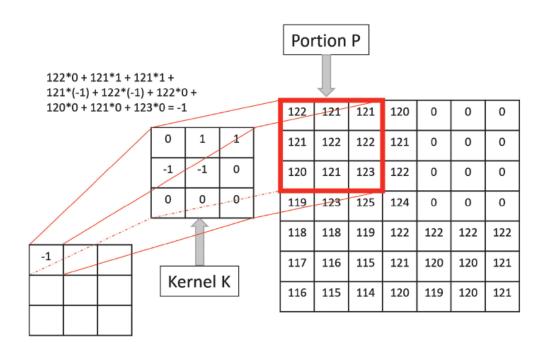
- Inspired by the organization of the visual cortex in the human brain, convolutional layers simulate the concept of a receptive field.
- Individual neurons in the convolutional layer respond only when a specific area of the image (the visual field) is active.
- An array of such neurons covers the entire image by responding to slightly overlapping separated areas of the input image.



Convolutional Neural Networks - CNN

- The idea of convolution relies on a kernel K, a mask to overlap onto a portion P of the image pixels for the convolution operation.
- From the product of the kernel K and the pixels in portion P we get a number, which will be the output of the first neuron in the convolutional layer.
- Then the kernel K moves n steps on the right and goes to cover another portion P of the image possibly slightly overlapping with the previous one; the output for the second unit of the convolutional layer is generated.
- And so on till the whole image has been covered by the kernel K and convoluted into output values.
- The distance in number of pixels n between two adjacent portions P is called stride.

Convolutional neurons: Example



Convolutional Neural Networks (CNN)

- Used when data has spatial relationships, e.g. images
- Instead of connecting every neuron to the new layer a sliding window is used
- Some convolutions may detect edges or corners, while others may detect cats, dogs, or street signs inside an image

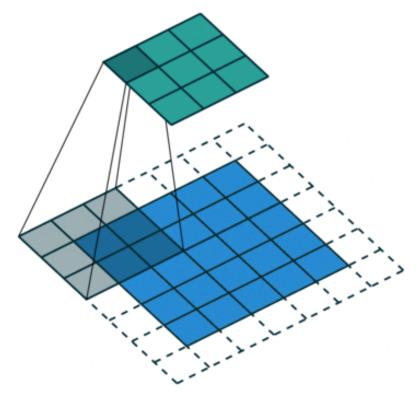


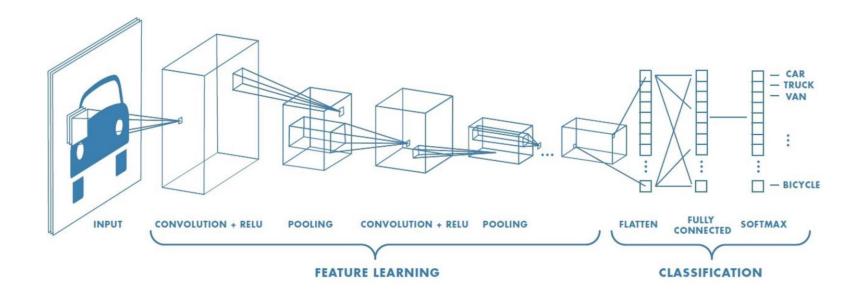
Image from: https://towardsdatascience.com/a-comprehensive-guide-to-convolutional-neural-networks-the-eli5-way-3bd2b1164a53

Pooling Layers

- Usually a number of convolutional layers are used.
- Each layer provides one further step in the process of extracting high-level features from the input image (colors, edges, entities, ...).
- After each convolutional layer, a pooling layer is often applied to reduce even further the data dimensionality.
- Two types of Pooling
 - Max Pooling returns the maximum value from the portion of the image covered by the Kernel.
 - Average Pooling returns the average of all values from the portion of the image covered by the Kernel.

Classification Layers

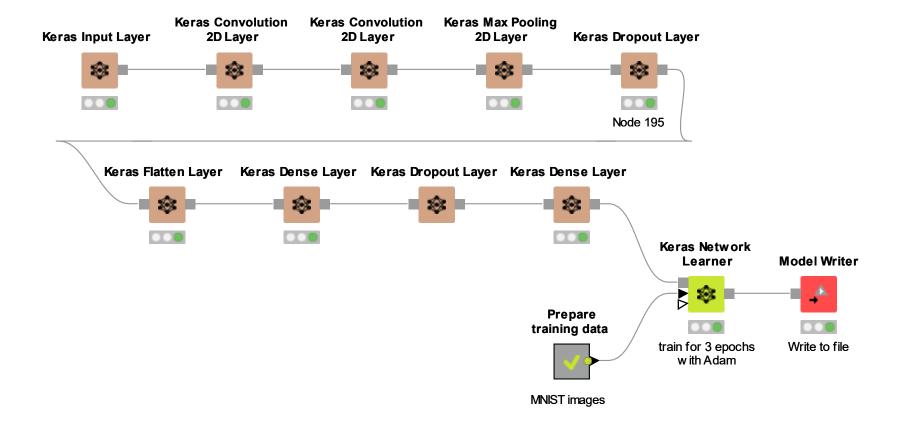
- After the sequence of convolutional + pooling layers, a classic feedforward multilayer Perceptron network is applied to carry out the classification process.
- Successful examples of CNNs for image recognition : LeNet, AlexNet, VGGNet, GoogLeNet, ResNet, ZFNet.



CNN: Transfer Learning

- Training such networks is a long and complex process, requiring very powerful machines.
- Instead of retraining a new network completely from scratch, we could recycle existing networks, already built and trained by others on similar data.
- This technique is called *Transfer Learning*.
- In Transfer Learning a model developed for a task is reused as the starting point for another model on a second task.
- On top of a previously trained network we add one or more neural layers
- We freeze all or some of the previously trained layers
- And we retrain only the remaining part of the whole network on our new task

Building CNNs with KNIME



Generative-Adversarial Networks (GANs)

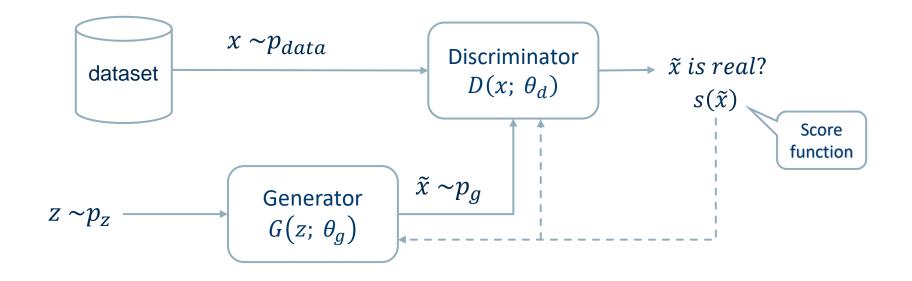
- So far: RNNs and CNNs
- Recurrent Neural Networks (RNNs) and Convolutional Neural Networks (CNNs) represent probably the biggest contribution of deep learning to the field of neural networks.
- However, deep learning is responsible for other innovations, such as for example Generative Adversarial Networks (GANs).

GAN: Generator

- GANs include two neural networks competing with each other: the generator and the discriminator.
- A **generator** G is a transformation that transforms the input noise z into a tensor usually an image x (x=G(z)). The generated image x is then fed into the discriminator network D.
- The discriminator network D compares the real images in the training set and the image generated by the generator network and produces an output D(x), which is the probability that image x is real.

GAN: Training

- Both generator and discriminator are trained using the backpropagation algorithm to produce D(x)=1 for the generated images x.
- Both networks are trained in alternating steps, competing with each other to improve themselves.
- The GAN model eventually converges and produces images that look real.
- Given a training set, this technique learns to generate new data under the same statistics as the training set.



GANs

- For example, a GAN trained on photographs can generate new photographs that look at least superficially authentic to human observers, having many realistic characteristics.
- GANs have been successfully applied to image tensors to create anime, human figures, and even van Gogh-like masterpieces.

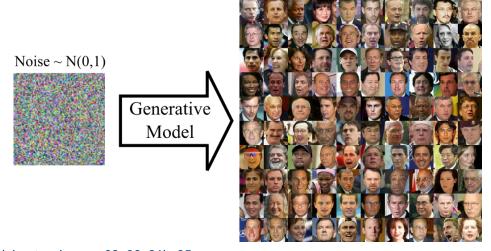


Image from: Pankaj Kishore, Towards data Science

https://towardsdatascience.com/art-of-generative-adversarial-networks-gan-62e96a21bc35

Practical Example

KNIME Workflows

 A multilayer perceptron with layers (4–8–3) is trained to classify the iris data set using the backpropagation algorithm, as set in the Keras Network Learner node

