Zurich University of Applied Sciences

NN for sequential data cntd.

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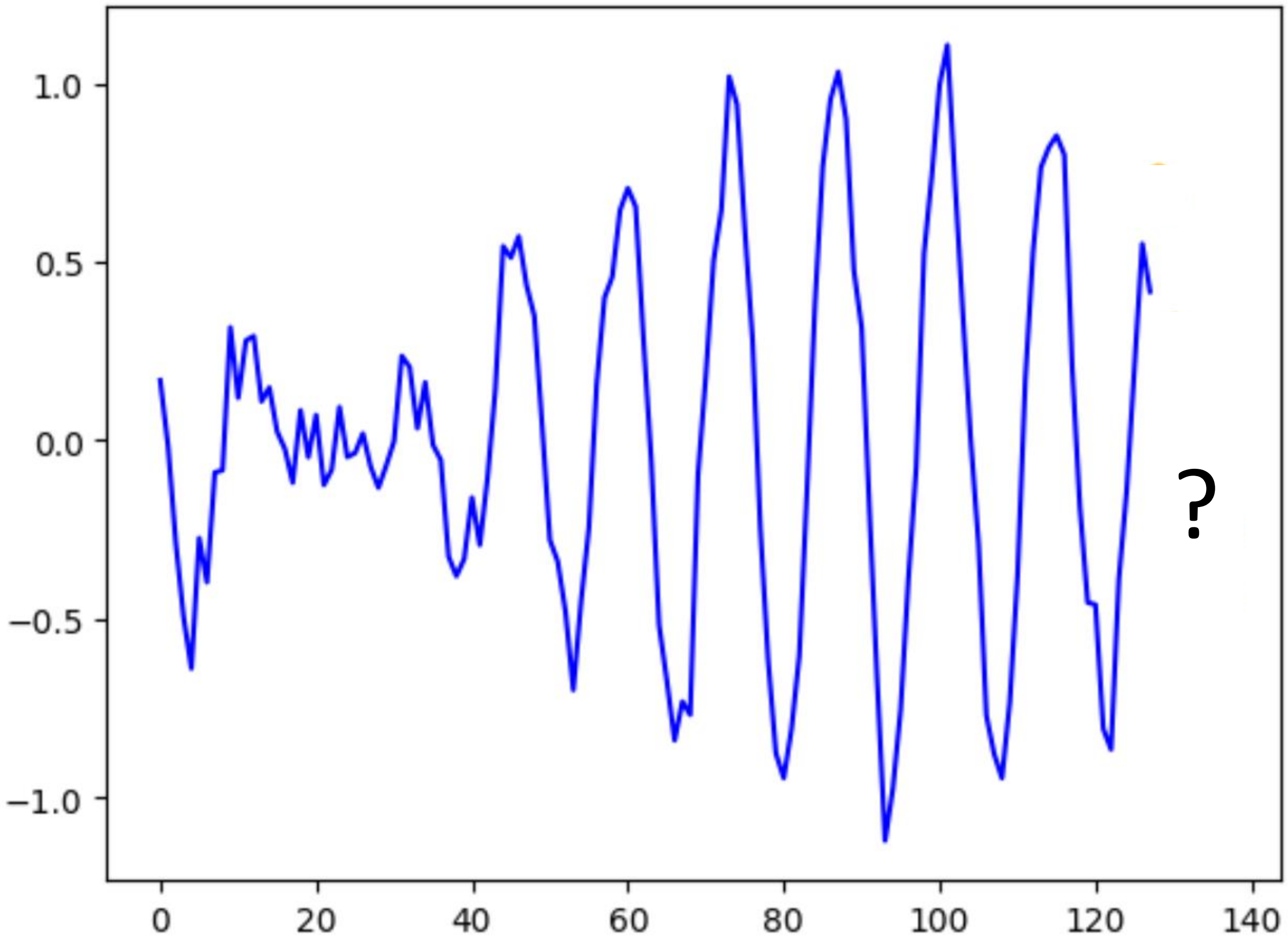
Remark: Much of the material has been developed together with Elvis Murina and Oliver Dürr

Topics

- **Recap architectures for sequential data**
  - 1D convolution
  - RNN

- **Recurrent NN with better memory**
  - GRU
  - LSTM

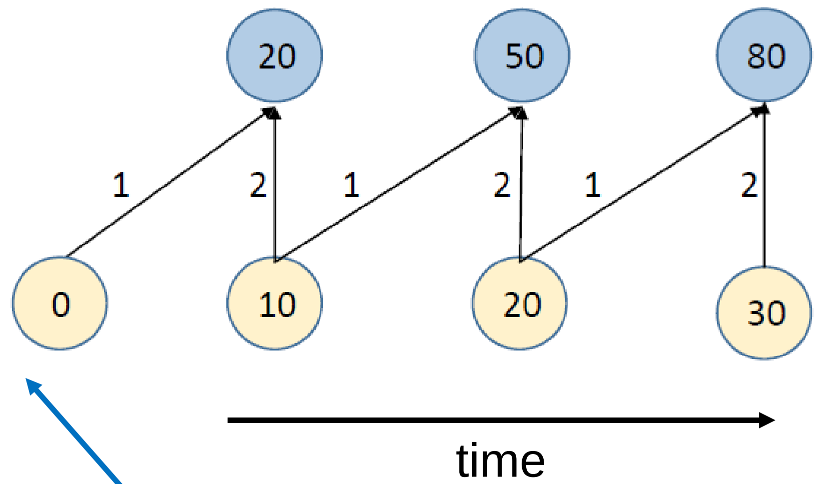
Task in homework: Predict how series will continue



Recap 1D "causal" convolution for ordered data

Toy example:

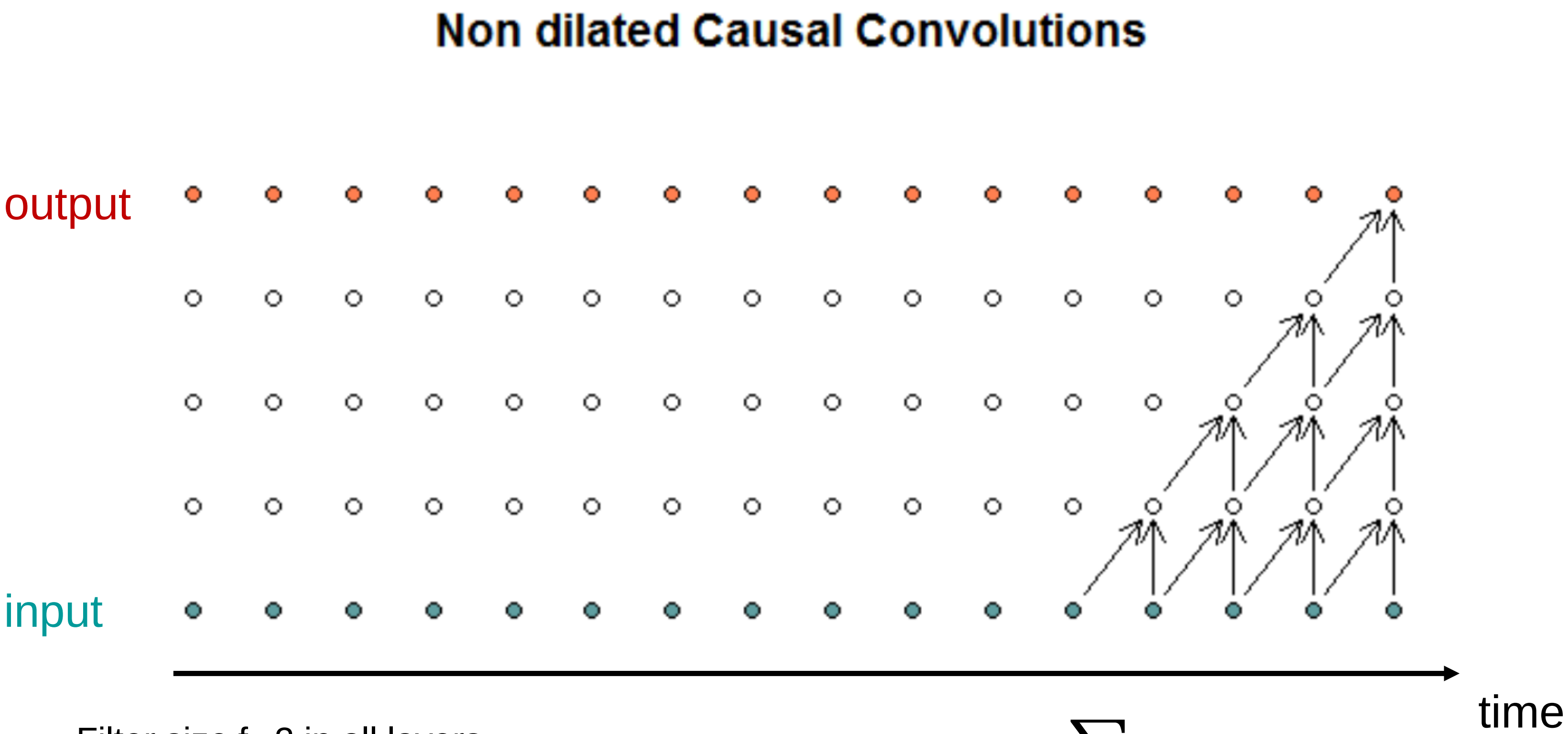
Output:	23	50	80
1D Kernel:	1	2	
Input	10	20	30



To make all layers the same size, a zero padding is added to the beginning of the input layers

"causal" networks, because the architecture ensured that no information from the future is used.

Stacking 1D "causal" convolutions without dilation



Filter size f_i=2 in all layers.
Hidden layers from i=1…3

$$ReceptiveField = f_0 + \sum_i (f_i - 1)$$

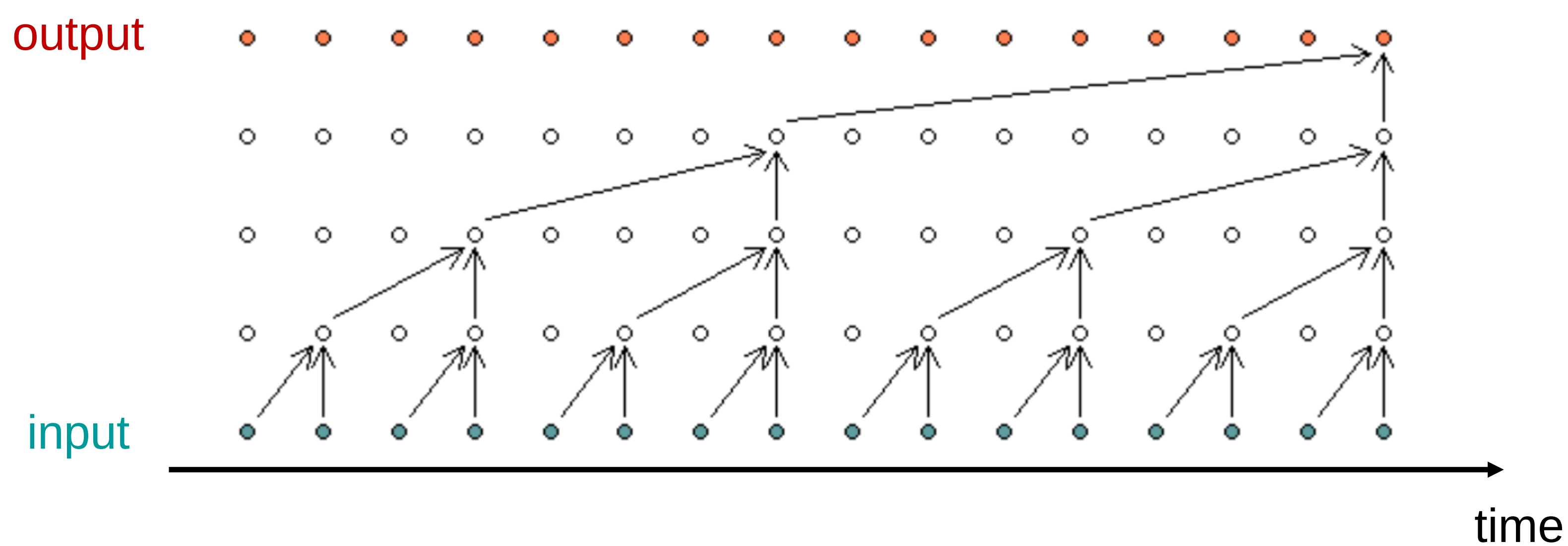
Stacking k causal 1D convolutions with kernel size 2 allows to look back k time-steps.

After 4 layers each neuron has a "memory" of 5 time-steps (1 presence and 4 past).

https://deepmind.com/blog/wavenet-generative-model-raw-audio/

Dilation allows to increase "memory" = receptive field

To increase the memory of neurons in the output layer, you can use "dilated" convolutions:



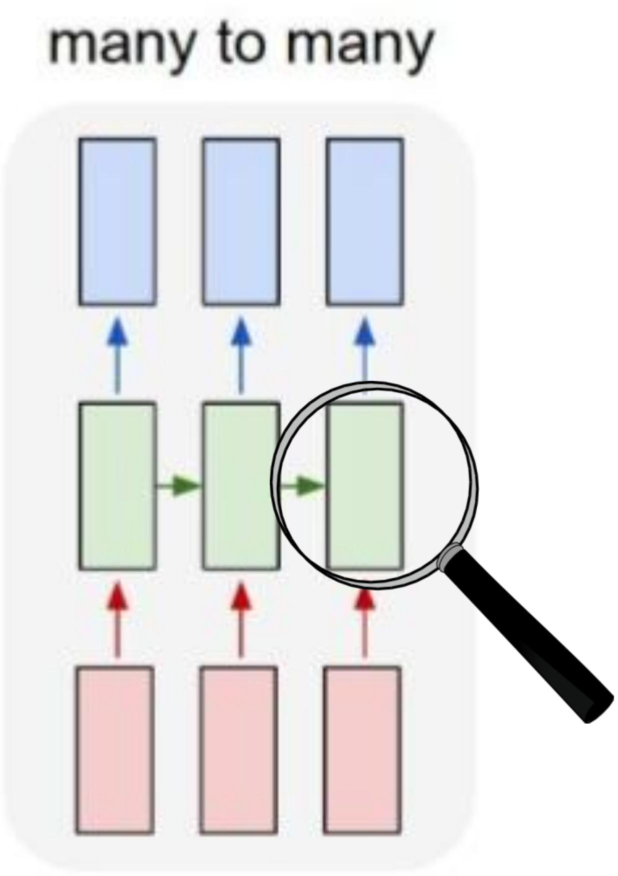
$$ReceptiveField = f_0 \cdot d_0 + \sum_i (f_i - 1) \cdot d_i \; = 2 \cdot 1 + 1 \cdot 2 + 1 \cdot 4 + 1 \cdot 8 = 16$$

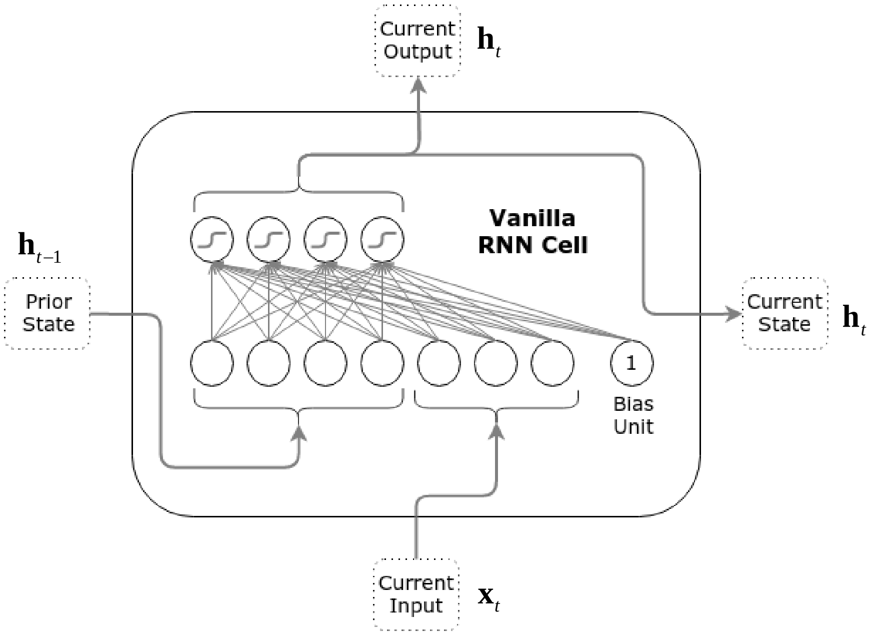
Here the filter f_i=2 for all layer, but dilation is d_i starts with 1 and doubles from layer to layer

After 4 layers each neuron has a receptive field of 16 input neurons.

https://deepmind.com/blog/wavenet-generative-model-raw-audio/
https://fomoro.com/projects/project/receptive-field-calculator Receptive field calculator

Recap the architecture of a simple RNN



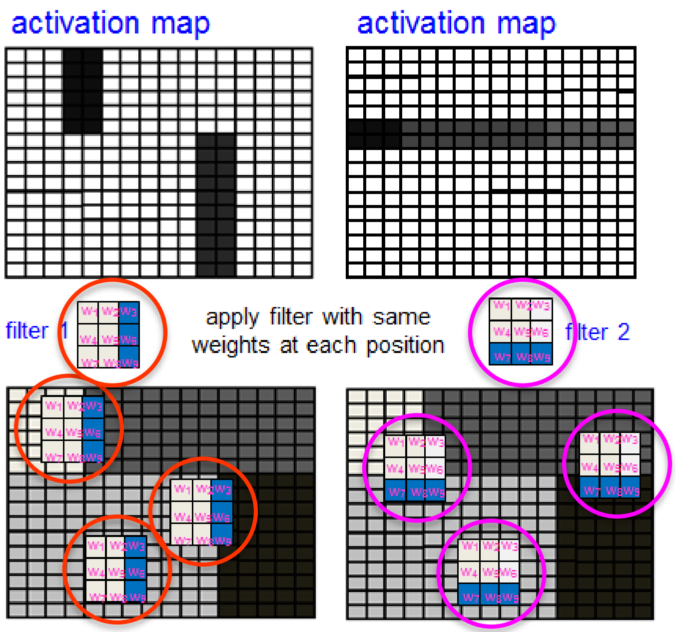


$$\text{output}=\mathbf{h}_t = \tanh\left([\mathbf{h}_{t-1}, \mathbf{x}_t]\cdot \mathbf{W} + \mathbf{b}\right)$$

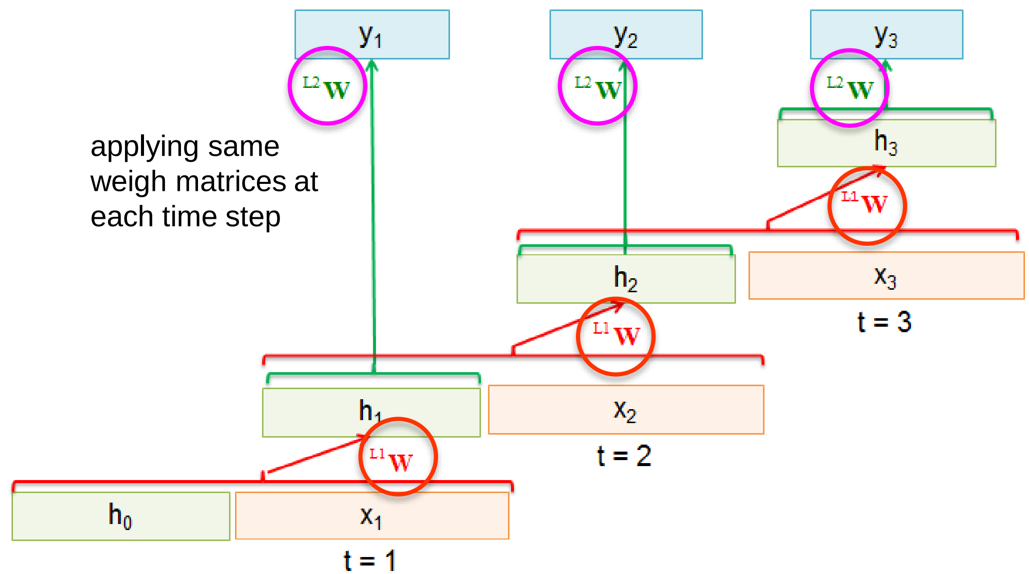
image credits: https://r2rt.com/written-memories-understanding-deriving-and-extending-the-lstm.html

Common tricks in RNN & CNN and some differences

CNN and Recurrent Network share weights



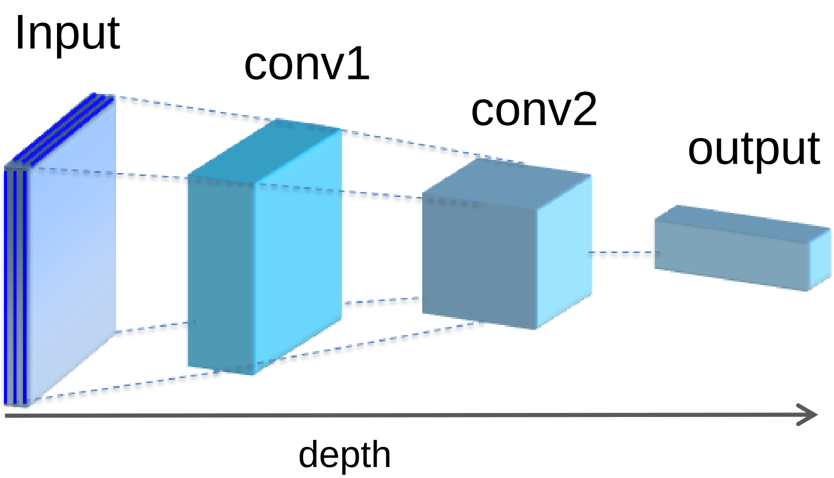
CNN share weights between different local regions of the image

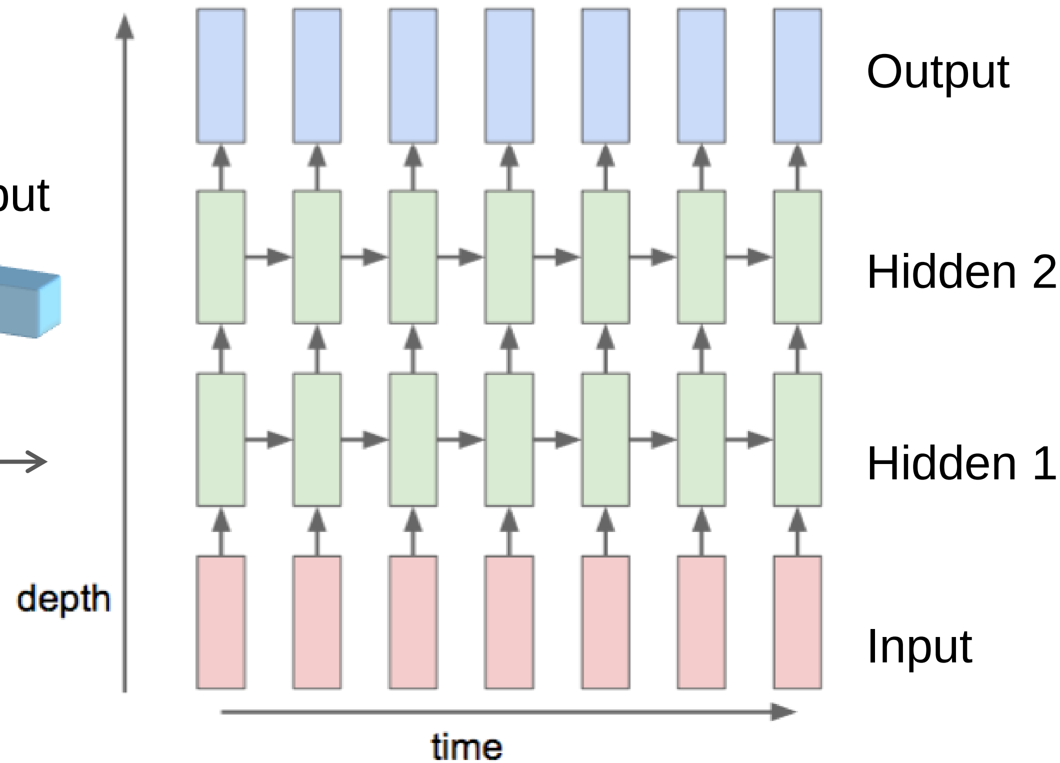


RNN share weights between time steps

Remark: no weight sharing in fully connected NN

Also in RNN we can go deep for hierarchical features

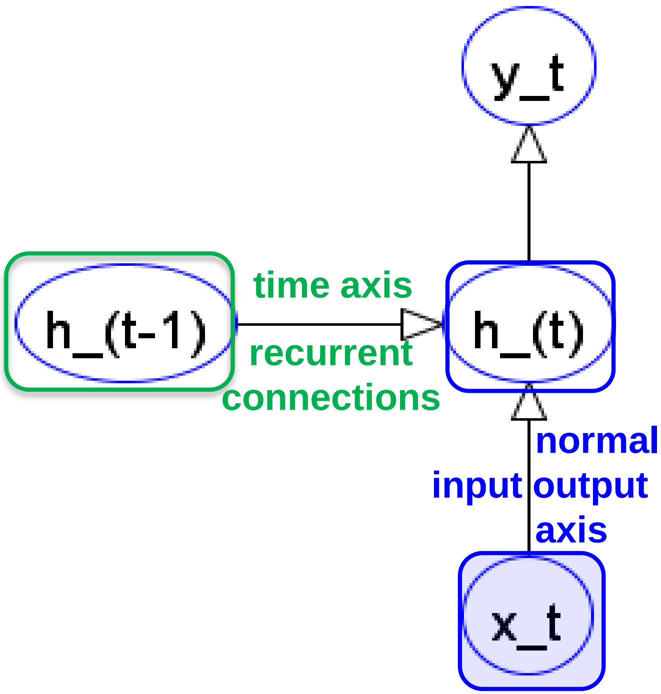


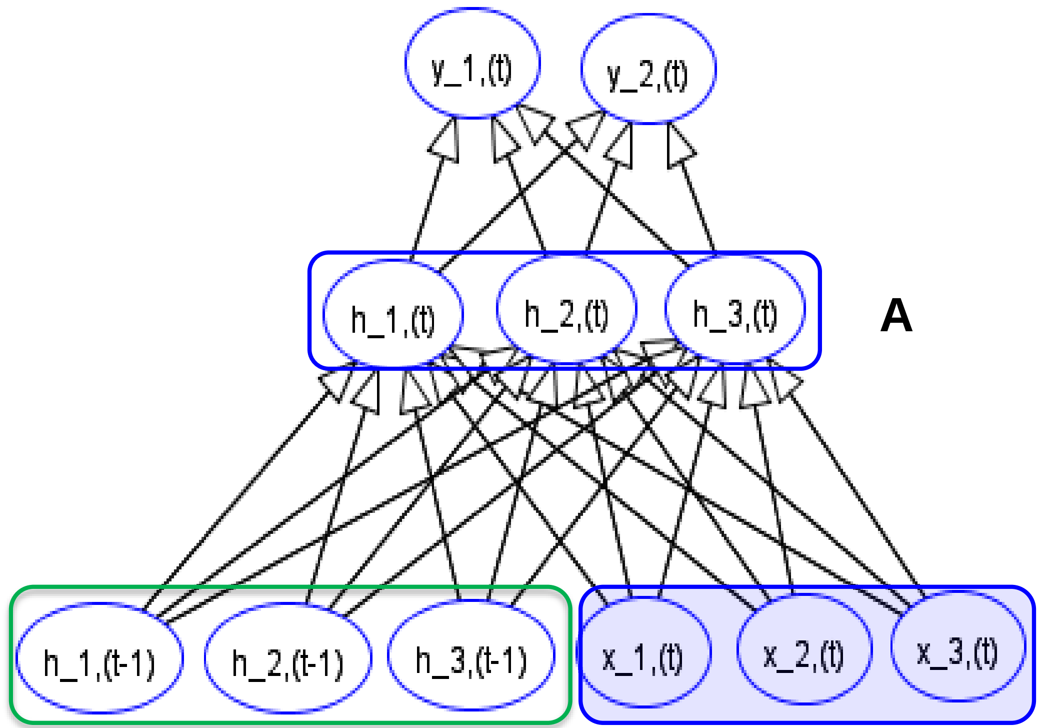


Usually we see only 1-4 hidden layers in an RNN compared to usually 4-100 stacked hidden convolutional blocks in CNNs.

Illustration: http://www.deeplearningbook.org/ and : http://karpathy.github.io/2015/05/21/rnn-effectiveness/

Dropout in recurrent architectures allow to choose different different dropout rates for recurrent and normal connections





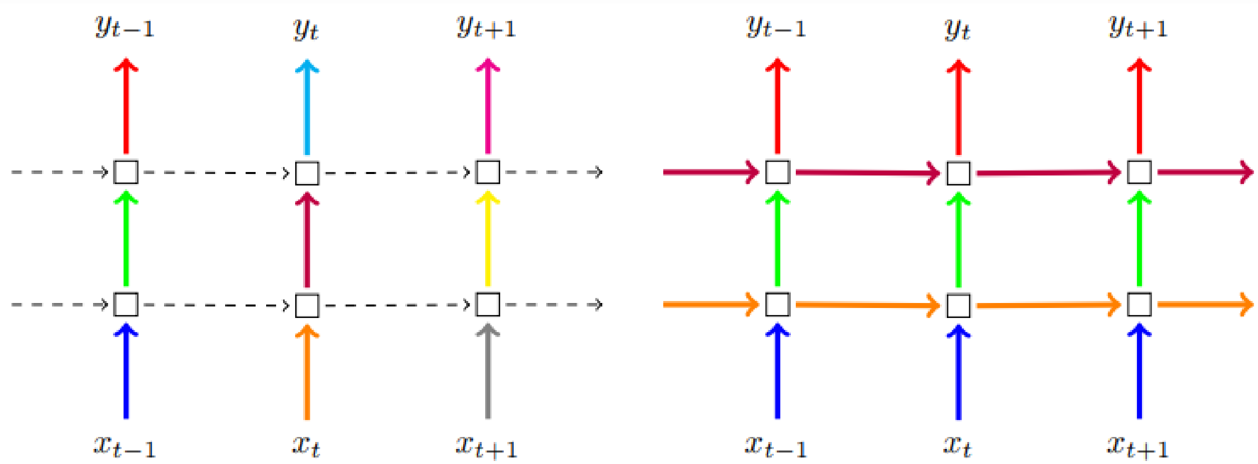
$$\mathbf{A} = f_{\mathbf{W}}(\mathbf{h}_{t-1}, \mathbf{x}_t) = \tanh\left([\mathbf{h}_{t-1}, \mathbf{x}_t] \cdot \mathbf{W} + \mathbf{b}\right) = \tanh\left(\mathbf{h}_{t-1} \cdot \mathbf{W}_h + \mathbf{x}_t \cdot \mathbf{W}_x + \mathbf{b}\right)$$

$$\mathbf{W} = \begin{pmatrix} \mathbf{W}_h \\ \mathbf{W}_x \end{pmatrix}$$

Dimensions in example: **W:**6x3, $\mathbf{W}_h$:3x3, $\mathbf{W}_x$:3x3

Dropout in recurrent architectures

It is important to use identical dropout masks (marked by arrows with same color) at different time steps in recurrent architectures like GRU or LSTM.



(a) Naive dropout RNN (b) Variational RNN

same arrow color indicates identical dropout mask

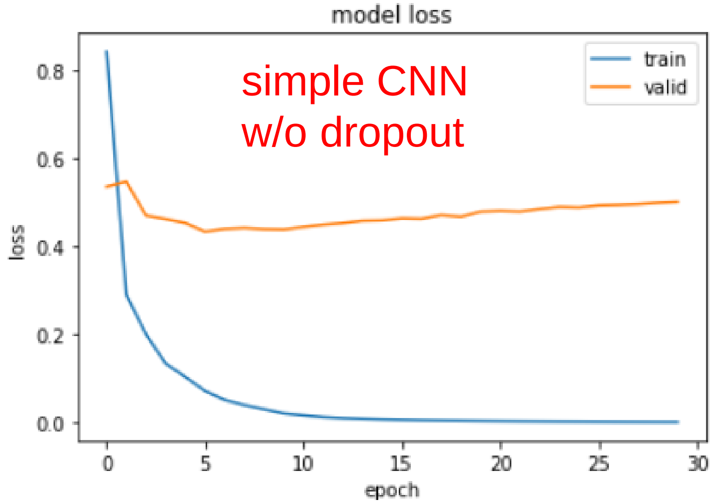
Figure 1: **Depiction of the dropout technique following our Bayesian interpretation (right) compared to the standard technique in the field (left).** Each square represents an RNN unit, with horizontal arrows representing time dependence (recurrent connections). Vertical arrows represent the input and output to each RNN unit. Coloured connections represent dropped-out inputs, with different colours corresponding to different dropout masks. Dashed lines correspond to standard connections with no dropout. Current techniques (naive dropout, left) use different masks at different time steps, with no dropout on the recurrent layers. The proposed technique (Variational RNN, right) uses the same dropout mask at each time step, including the recurrent layers.

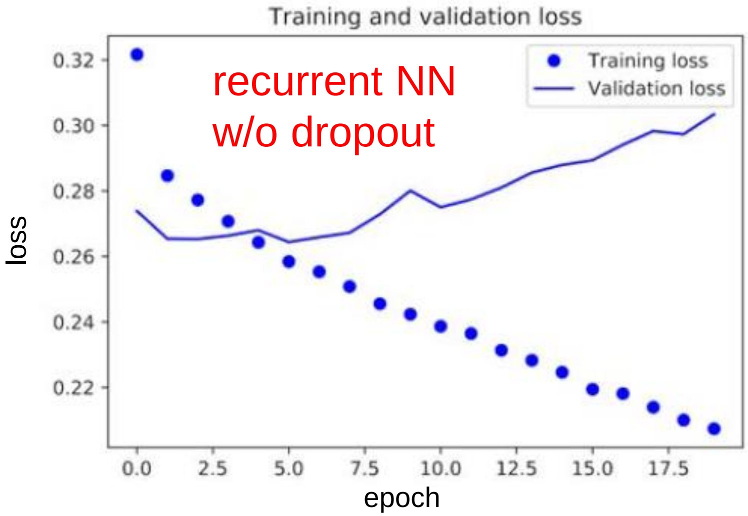
[Gal2016]

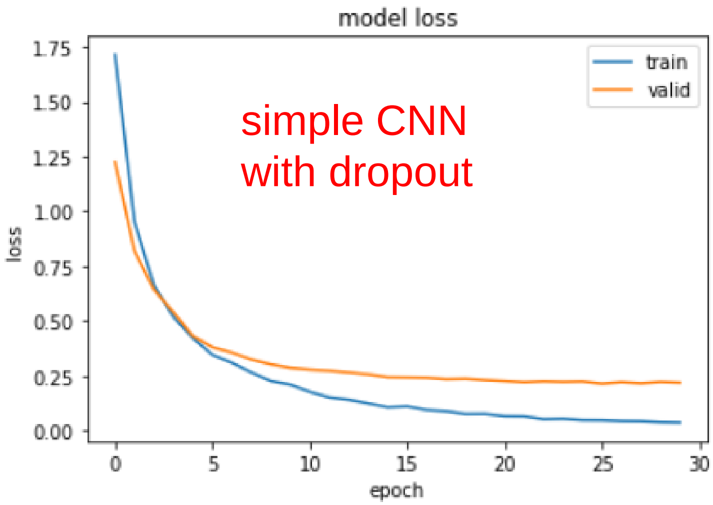
In keras:

```
model.add(layers.GRU(32, dropout=0.2, recurrent_dropout=0.2, input_shape=(None, …)))
```

Dropout can fight overfitting in CNN and recurrent NN







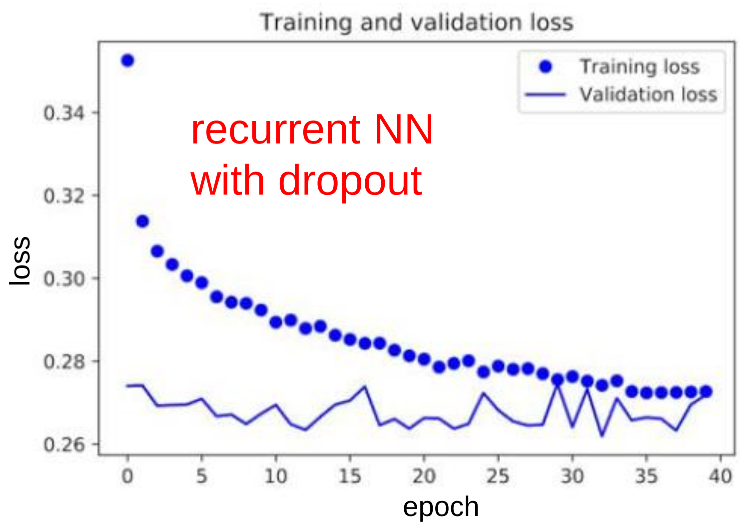
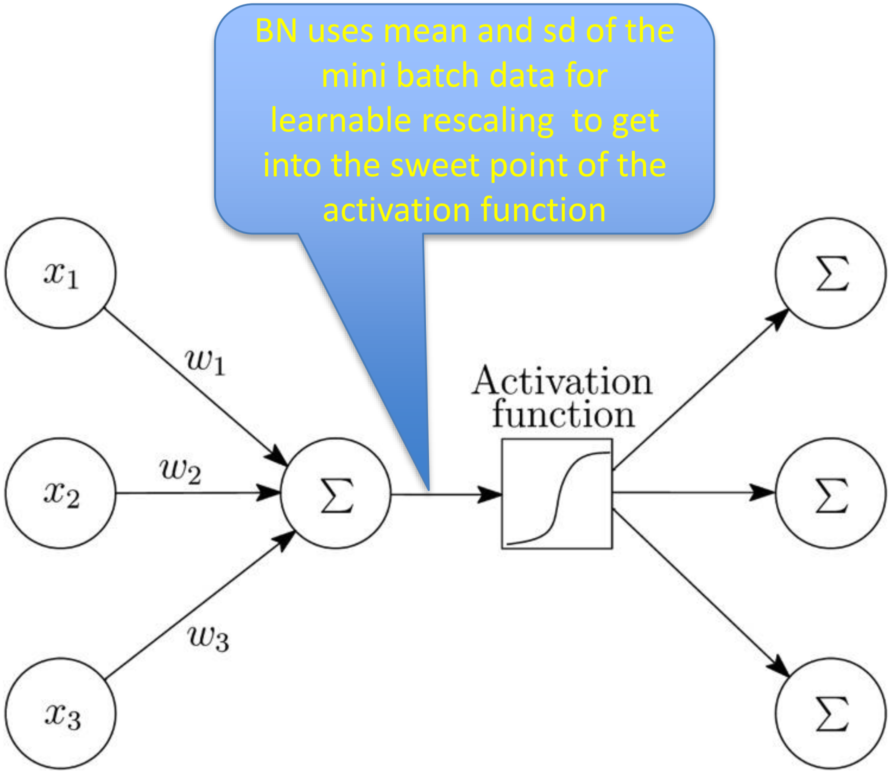
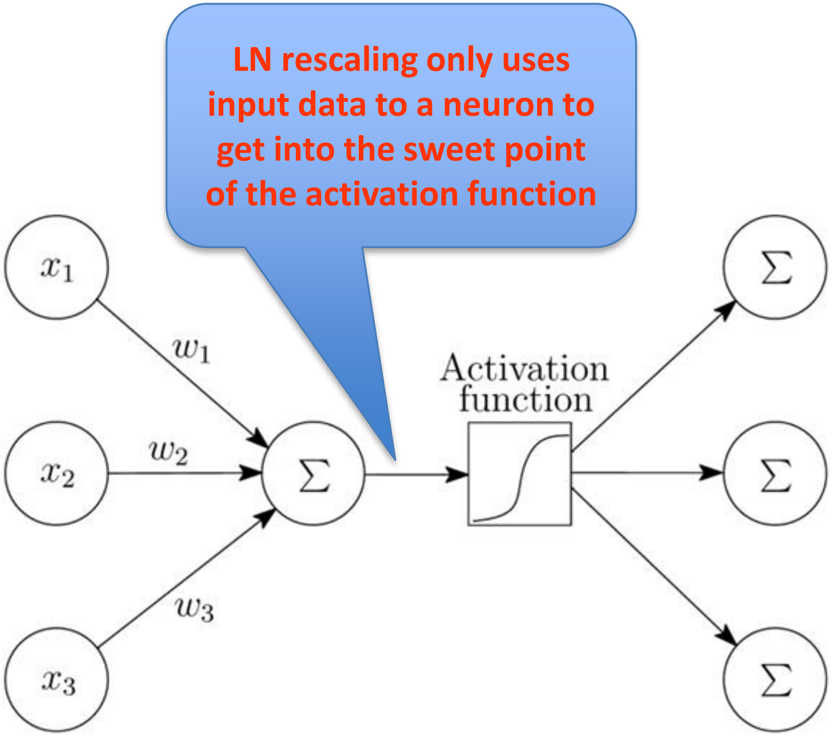


Image credits: F Chollet's book: DL with Python

Batchnormalization is crucial to train deep CNNs
Layernormalization is benefial in RNN: LN $\neq$ BN





Applying BN to RNN would not take into account the recurrent architecture of the NN over which statistics of the input to a neuron might change considerable within the same mini batch. In LN the mean and variance from all of the summed inputs to the neurons in a layer on a single training case are used for normalization .

For details on layer nomarlization see [Ba.Kiros.Hinton2016]

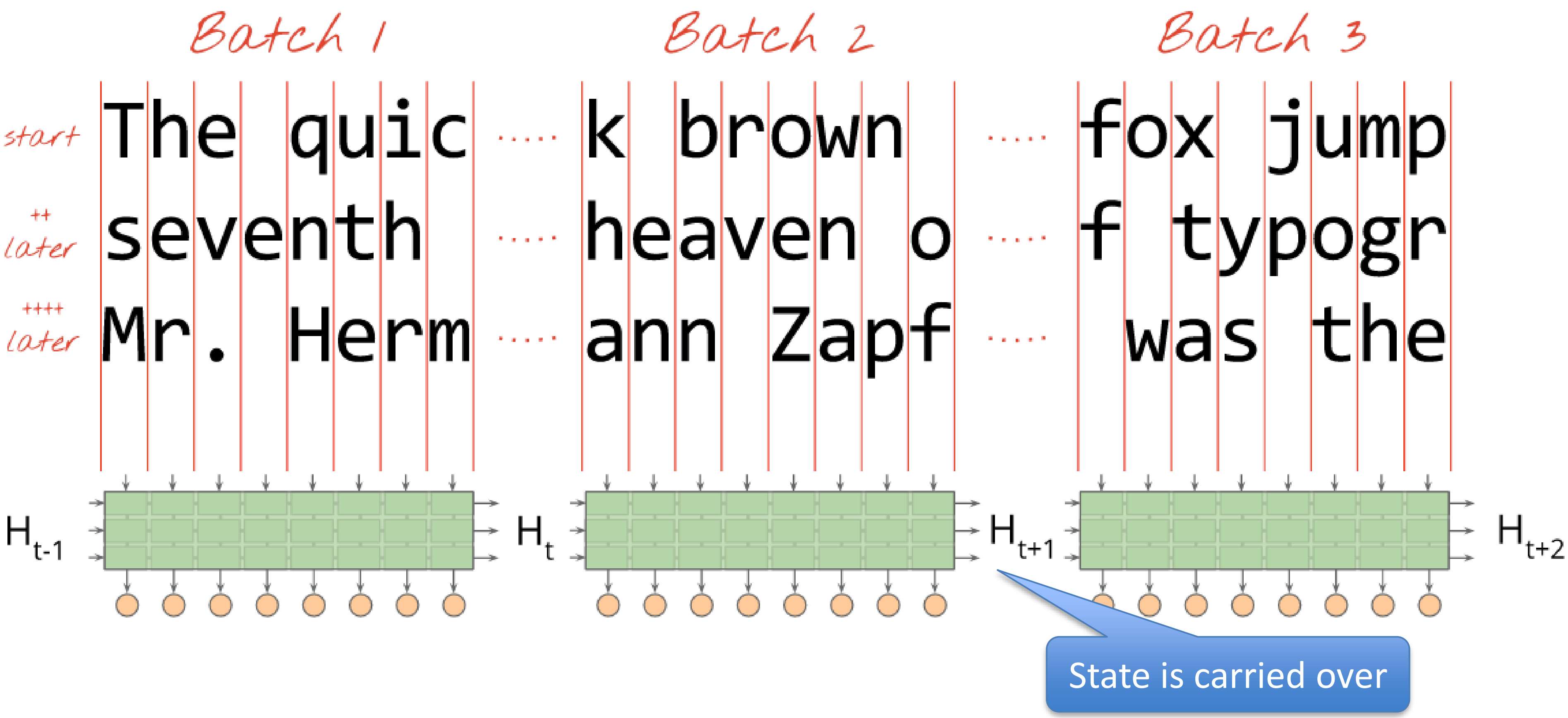
Stateful RNN model

Training a stateful RNNs

- RNN are often trained on sequence data with inherent order
- Sequences are often very long and need to be cut between mini-batches
- By default the hidden state is initialized with zeros in each mini-batch
- In stateful RNN we connect sequences in the right order between mini-batches allowing to make use of the hidden state learned so far
- This requires a careful construction of the mini-batches and an appropriate transfer of the hidden state between mini-batches

Mini-batches in statefull RNN

The gradient is propagated back a fixed amount of steps defined by the size of a mini-batch. In stateful RNNs the hidden state is carried over between mini-batches and hence between connecting sequences given appropriate batches.



Slide credit Martin Gorner (TensorFlow without PhD)

Vanishing/Exploding Gradient problem during training a RNN

Recall: Loss of a mini-batch is used to determine update

mini-batch of size M=8

train data input (S=len(seq)=3):

instance_id	seq_t1	seq_t2	seq_t3
1	$\mathbf{x}_{11}$	$\mathbf{x}_{12}$	$\mathbf{x}_{13}$
2	$\mathbf{x}_{21}$	$\mathbf{x}_{22}$	$\mathbf{x}_{23}$
3	$\mathbf{x}_{31}$	$\mathbf{x}_{32}$	$\mathbf{x}_{33}$
⋮	⋮	⋮	⋮
8	$\mathbf{x}_{81}$	$\mathbf{x}_{82}$	$\mathbf{x}_{83}$

train data target (2 classes, K=2):

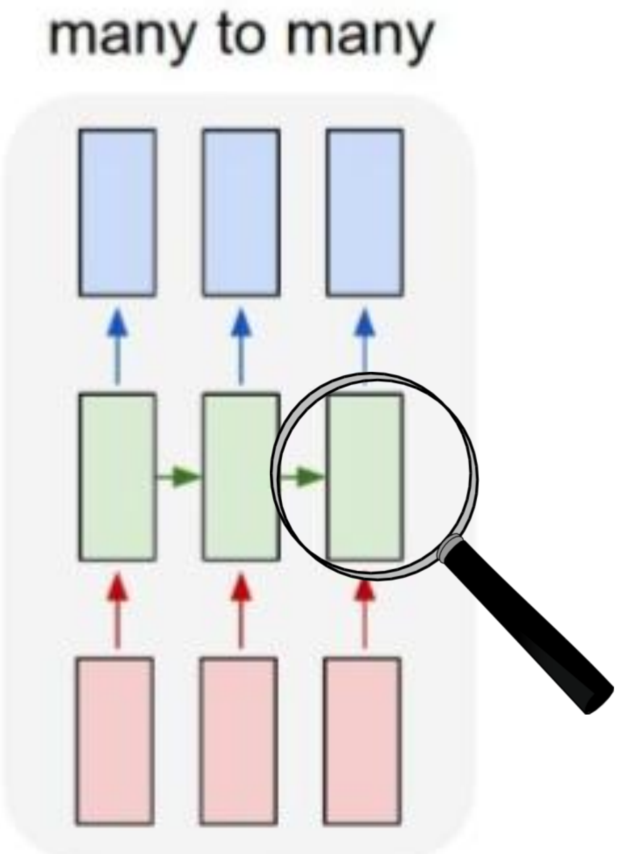
instance_id	y_t1	y_t2	y_t3
1	(1,0)	(1,0)	(0,1)
2	(0,1)	(1,0)	(0,1)
3	(0,1)	(0,1)	-1
⋮	⋮	⋮	⋮
8	(1,0)	(1,0)	(1,0)

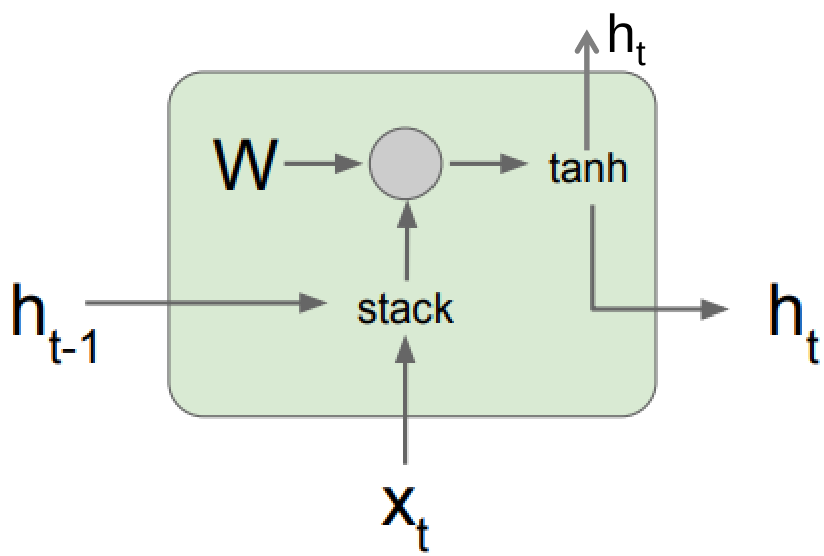
Cost C or Loss is given by the cross-entropy averaged over all instances in mini-batch:

$$\text{Loss} = \frac{1}{8}\sum_{m=1}^{8}\left[\sum_{s=1}^{3}\left(-\sum_{k=1}^{2} y_{\text{msk}} \cdot \log\left(p_{\text{msk}}\right)\right)\right]$$

Based on the mini-batch loss the weights in the tow weight matrices of layer 1 and layer 2 are updated.

Recall: Design of a RNN "cell"

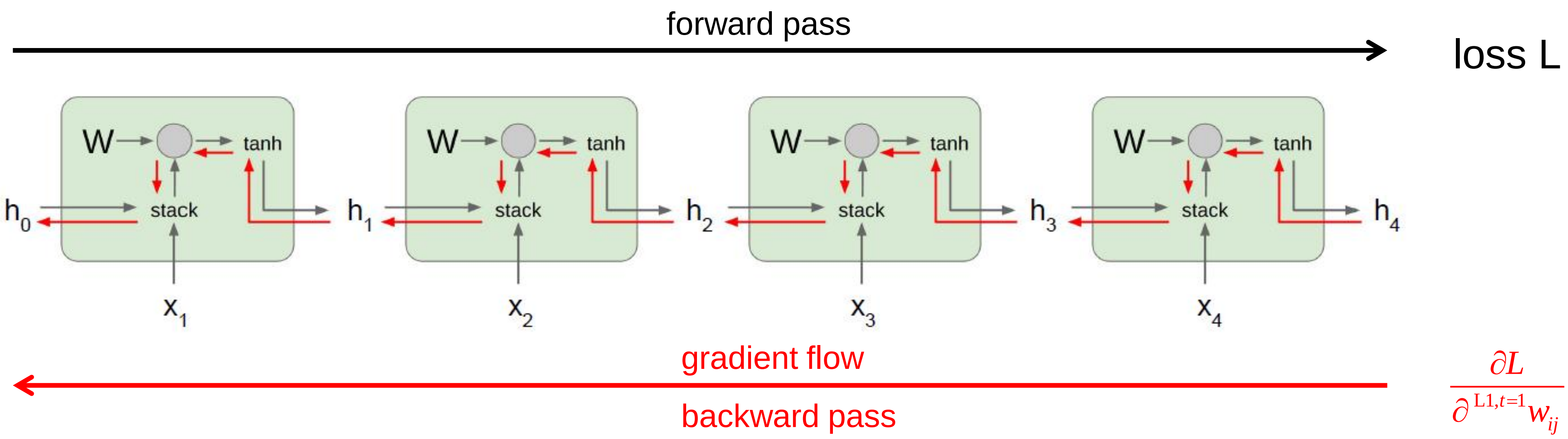




parameter?

$$(|h| + |x|) \cdot |h| + |h$$

Backpropagation in RNNs: Gradient is multiplied at each time step with same factor: Gradient explosion/vanishing



Propagating the gradient of the cost function via chain rule to the first time point involves multiplying at each time step with $\mathbf{W}^T$ (and the derivation of tanh).

⟹ Vanishing gradient if we multiply at each time step with a number <1
(more precisely we have only a number if W is a scalar, otherwise we need to look on the first singular value of $\mathbf{W}^T$)

⟹ Exploding gradient if we multiply at each time step with a number >1
(more precisely we have only a number if W is a scalar, otherwise we need to look on the first singular value of $\mathbf{W}^T$)

Solution: gradient clipping (hack), or use better architecture like LSTM or GRU!

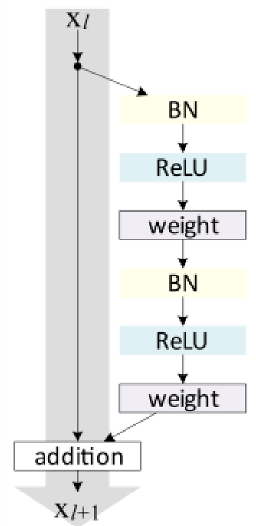
slide (adapted) from cs231 lecture 10

GRU and LSTM cells to avoid vanishing/exploding gradients

Recall: ResNet

- use ResNet like architectures allowing for a gradient highway

(in CNN also batch-normalization and ReLU helped to train deep NN, but cannot naively transfered to recurrent NN)



ResNet basic design (VGG-style)

- add shortcut connections every two
- all 3x3 conv (almost)

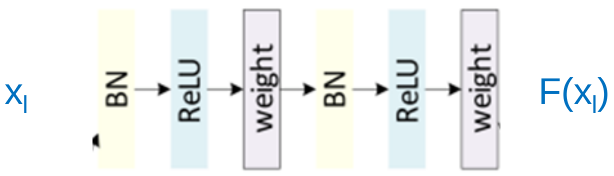
152 layers:
Why does this train at all?

This deep architecture could still be trained, since the gradients can skip layers which diminish the gradient!

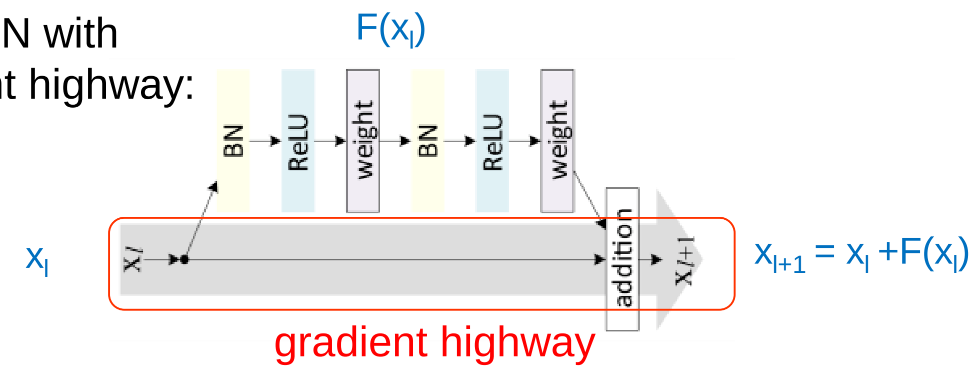
$$x_{l+1} = x_l + F(x_l)$$

Provide gradient highway also in recurrent NN: GRU, LSTM

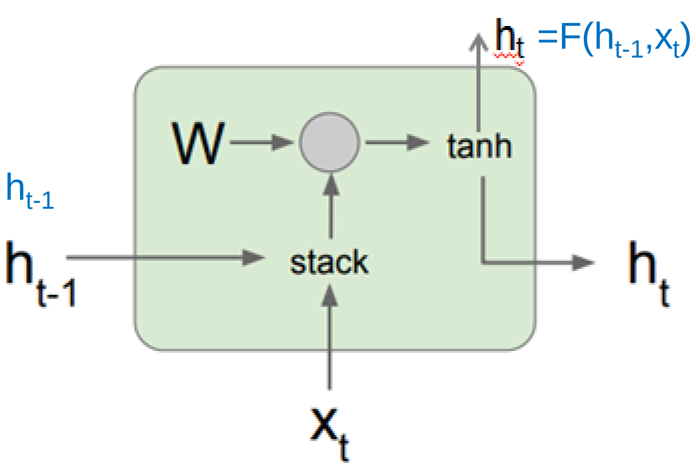
CNN classic:



CNN with gradient highway:

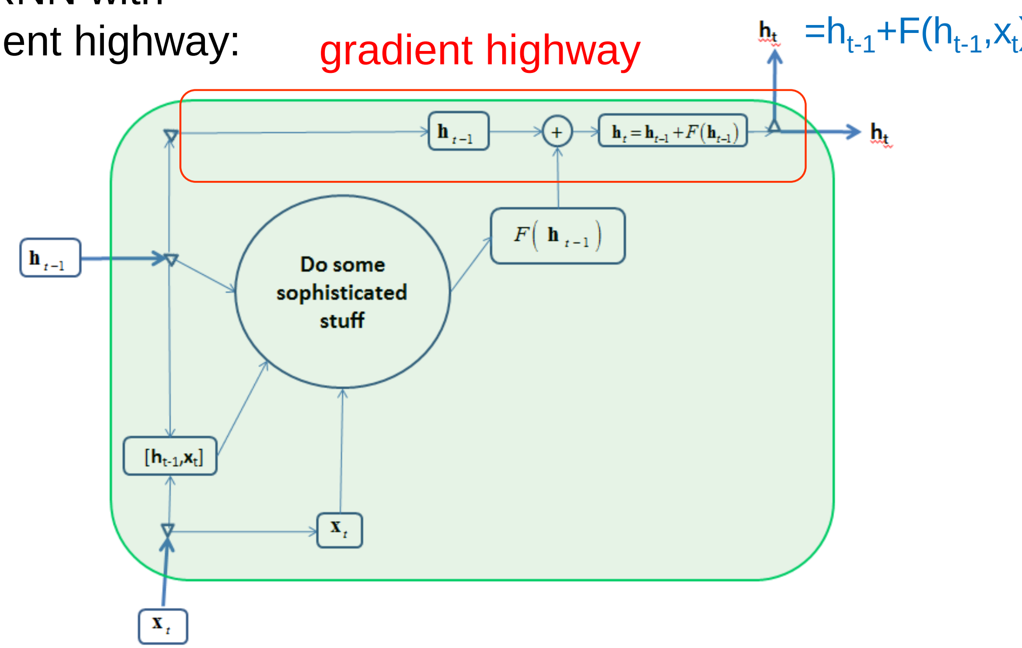


RNN classic:

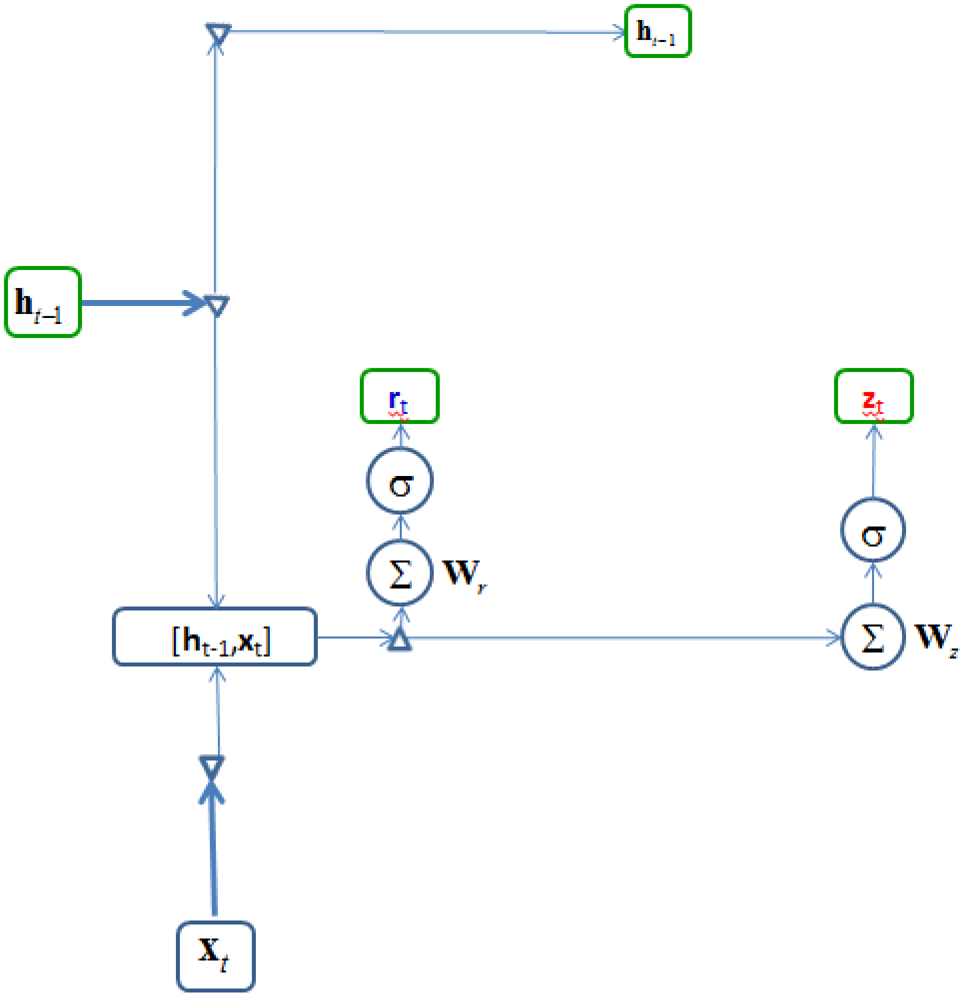


$$\mathbf{h}_t = \tanh\left([\mathbf{h}_{t-1}, \mathbf{x}_t] \cdot \mathbf{W} + \mathbf{b}\right)$$

RNN with gradient highway:



Towards Gated Recurrent Units (GRU)



$$\mathbf{r}_t = \text{gate}_{r,t} = \text{sigmoid}\left([\mathbf{h}_{t-1}, \mathbf{x}_t] \cdot \mathbf{W}_r + \mathbf{b}_r\right)$$

$$\mathbf{z}_t = \text{gate}_{\text{update}} = \text{sigmoid}\left([\mathbf{h}_{t-1}, \mathbf{x}_t] \cdot \mathbf{W}_z + \mathbf{b}_z\right)$$

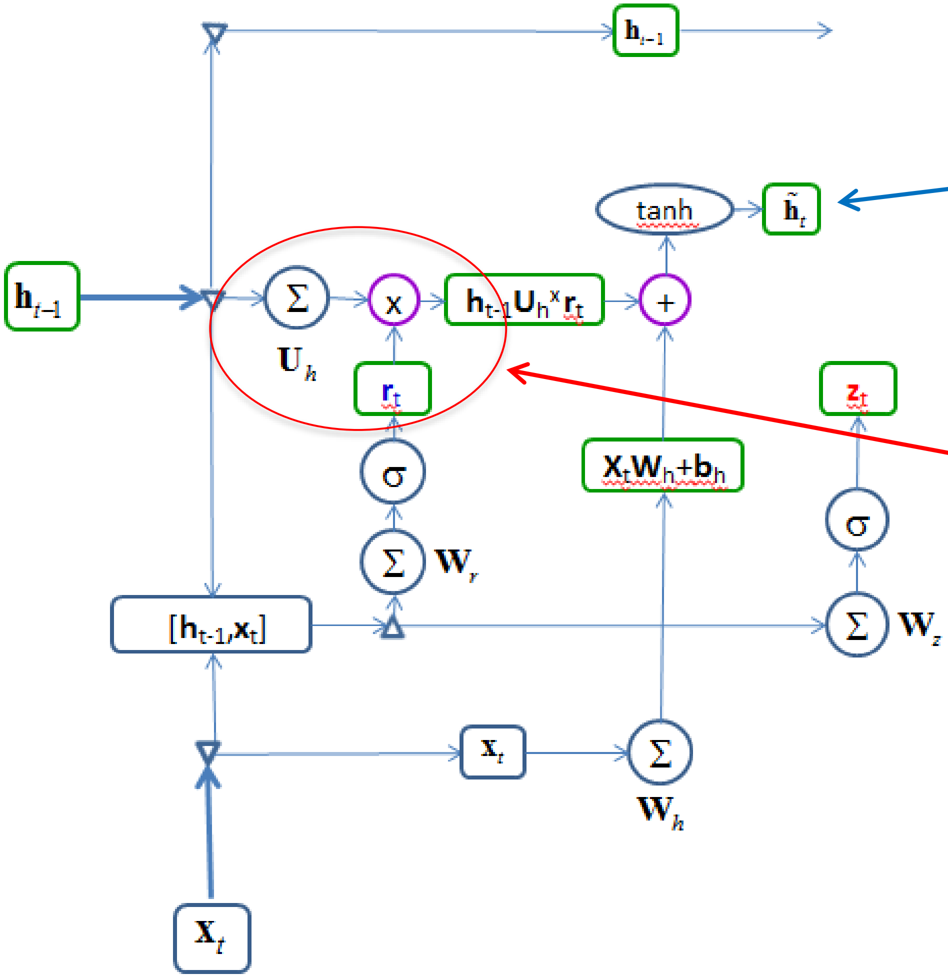
Idea:

The **relevant gate r** controls which part of the previous hidden state is relevant for making a prediction or should be dropped

The **updated gate z** controls how much information from the previous hidden layer h_{i-1} and the new input should be propagated to the current hidden layer h_i.

Remark: all internal vectors/tensors with green frame have same length/shape.

Towards Gated Recurrent Units (GRU)



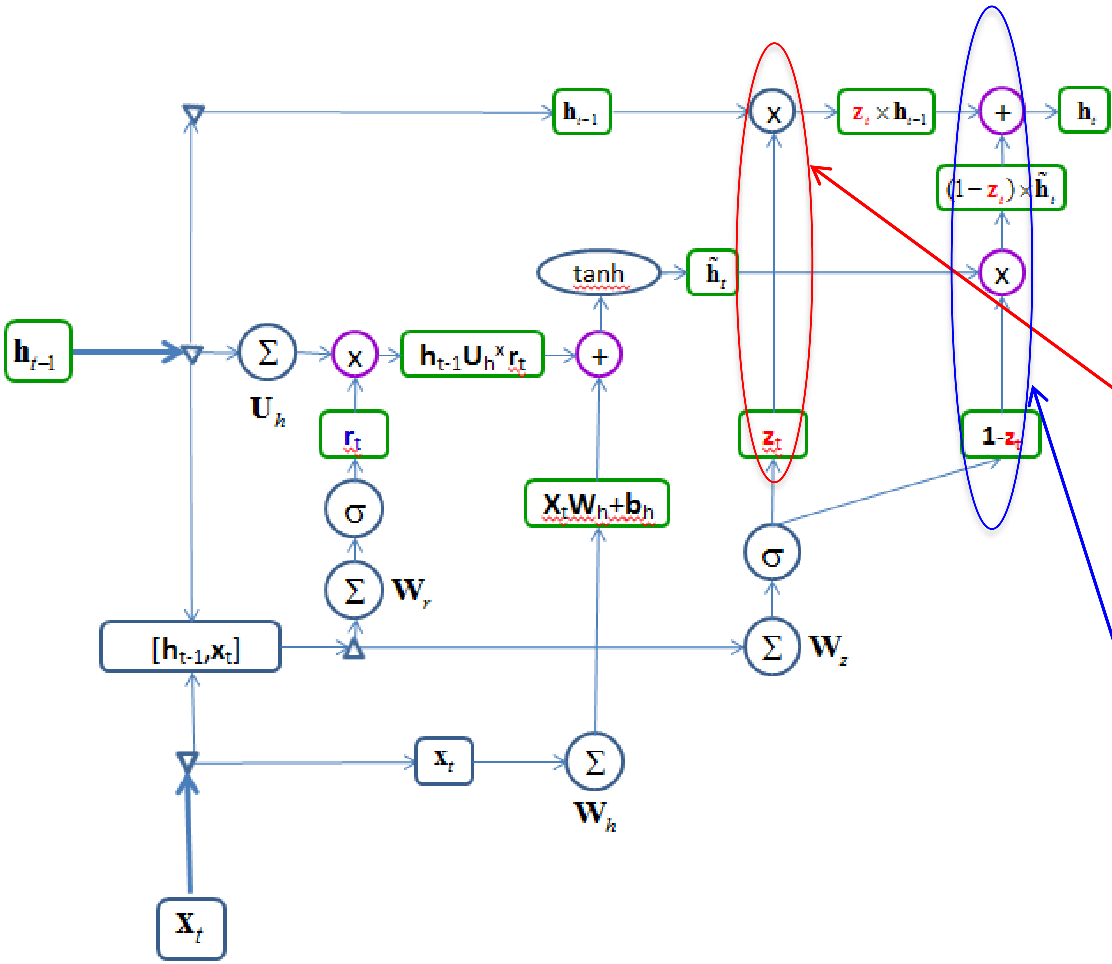
The new proposed state $\tilde{h}$ is:

$$\tilde{\mathbf{h}}_t = \tanh\left(\mathbf{x}_t \cdot \mathbf{W}_h + \mathbf{b}_h + \underline{\mathbf{h}_{t-1}\mathbf{U}_h \otimes \mathbf{r}_t}\right)$$

Here, we use the relevant gate r to control what part of $\boldsymbol{h_{t-1}}$ we need to compute a new proposal.

Remark: all internal vectors with green frame have same length.
All ops within a purple circle are performed per element-wise on the ingoing vectors

The Gated Recurrent Unit (GRU)



The new hidden state is:

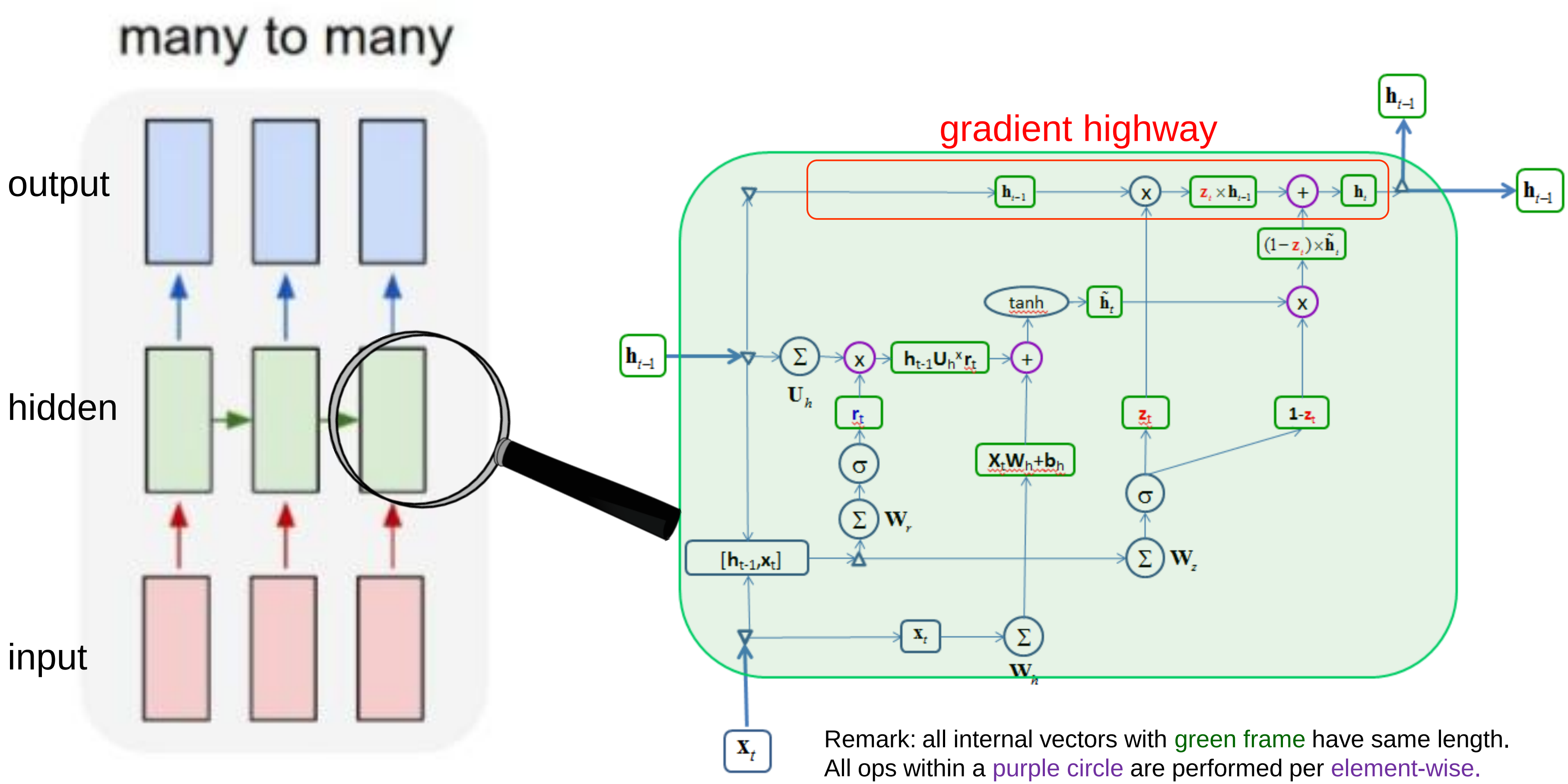
$$h_t = (1-z_t) \otimes \tilde{h}_t \oplus z_t \otimes h_{t-1}$$

If all elements of $\mathbf{z}_t$ are 1 then the hidden state stays unchanged.

The updated gate $\mathbf{z}_t$ controls how much of the previous hidden state $\mathbf{h}_{t-1}$ and the new input $\mathbf{x}_t$ should be propagated to the current hidden state $\mathbf{h}_t$

The updated gate $\mathbf{z}_t$ controls also how much information from proposed new state $\tilde{h}$ is entering the new state

Solution via "highway allowing" architecture: GRU

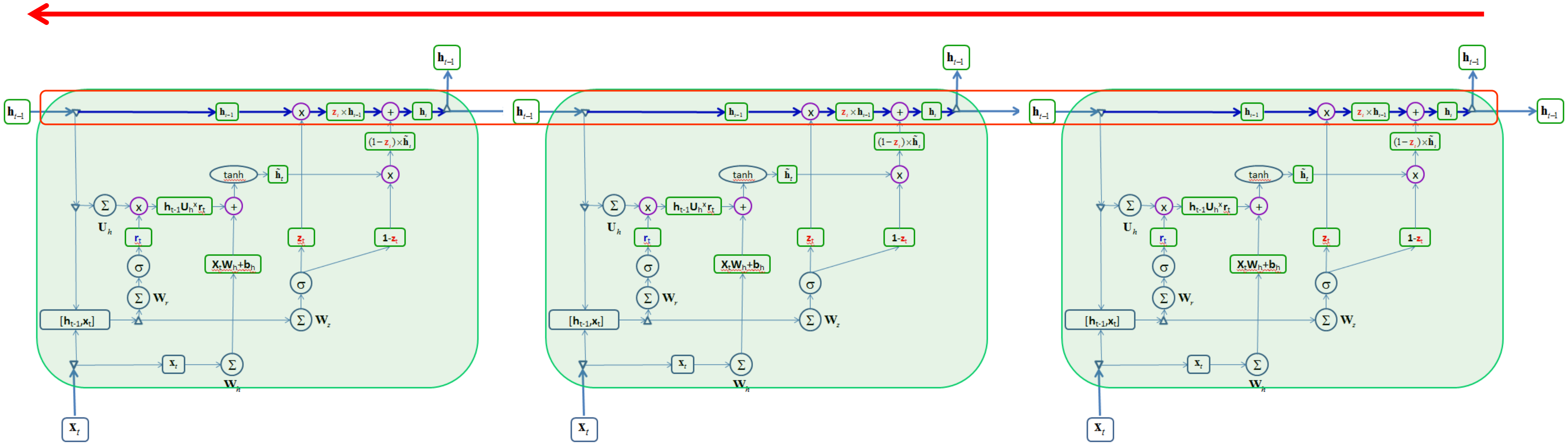


Remark: all internal vectors with green frame have same length.
All ops within a purple circle are performed per element-wise.

The gradient high-way avoids gradient vanishing. The GRU also avoids gradient explosion since the element-wise operations on vector-elements that change over the time steps, avoids multiplying the gradients with the same number in each step.

The Gated Recurrent Unit (GRU): Gradient Flow

Uninterrupted gradient flow!



parameter?

Relevant gate: $\mathbf{r}_t = \sigma\left([\mathbf{h}_{t-1}, \mathbf{x}_t] \cdot \mathbf{W}_r + \mathbf{b}_r\right)$

Update gate: $\mathbf{z}_t = \sigma\left([\mathbf{h}_{t-1}, \mathbf{x}_t] \cdot \mathbf{W}_z + \mathbf{b}_z\right)$

Proposed hidden state: $\tilde{\mathbf{h}}_t = \tanh\left(\mathbf{x}_t \cdot \mathbf{W}_h + \mathbf{b}_h + \mathbf{h}_{t-1}\mathbf{U}_h \otimes \mathbf{r}_t\right)$

New hidden state is: $\mathbf{h}_t = (\mathbf{1}\text{-}\mathbf{z}_t) \otimes \tilde{\mathbf{h}}_t \oplus \mathbf{z}_t \otimes \mathbf{h}_{t-1}$

$$(|h| + |x|) \cdot |h| + |h$$

$$+(|h| + |x|) \cdot |h| + |h|$$

$$+ \; (|x|) \cdot |h| + |h| + \; (|h|) \cdot |h|$$

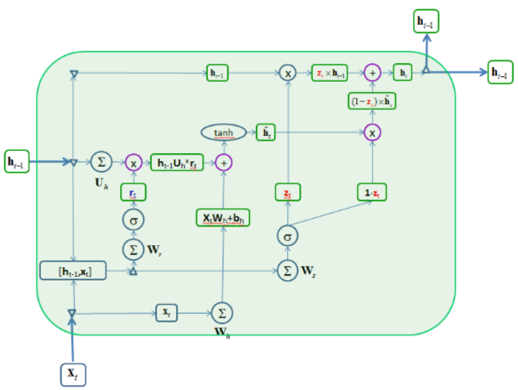
$$= 3 \cdot [(|h| + |x|) \cdot |h| + |h|]$$

A simplified variation, the Gated Recurrent Unit, or GRU, introduced by Cho, et al. (2014).

GRU in keras

```
from keras.models import Sequential
from keras import layers
from keras.optimizers import RMSprop

model = Sequential()
model.add(layers.GRU(32, input_shape=(None, float_data.shape[-1])))
model.add(layers.Dense(1))

model.compile(optimizer=RMSprop(), loss='mae')
history = model.fit_generator(train_gen,
                              steps_per_epoch=500,
                              epochs=20,
                              validation_data=val_gen,
                              validation_steps=val_steps)
```

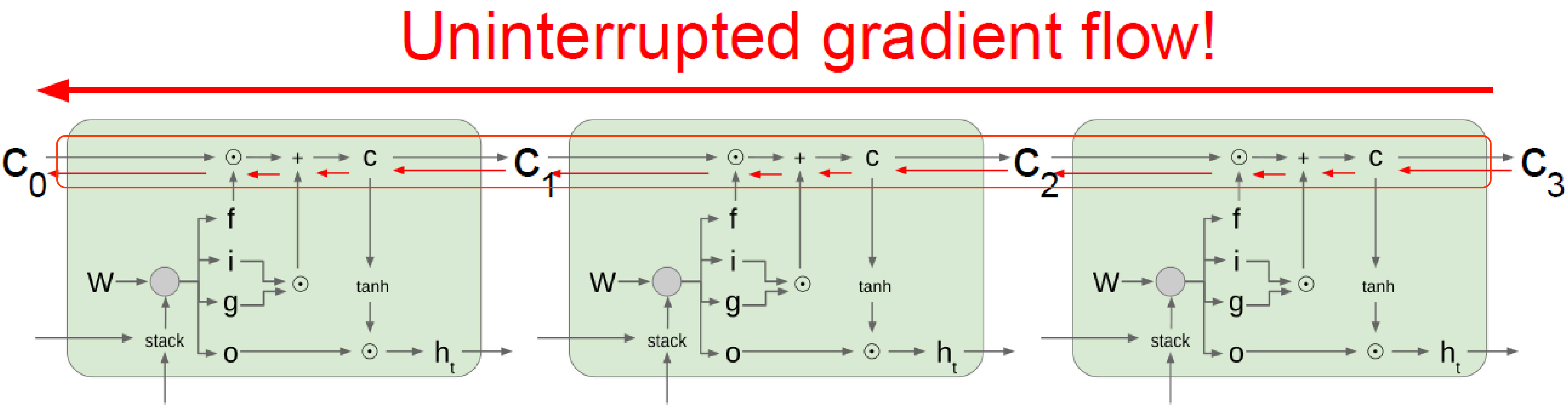
length of internal state



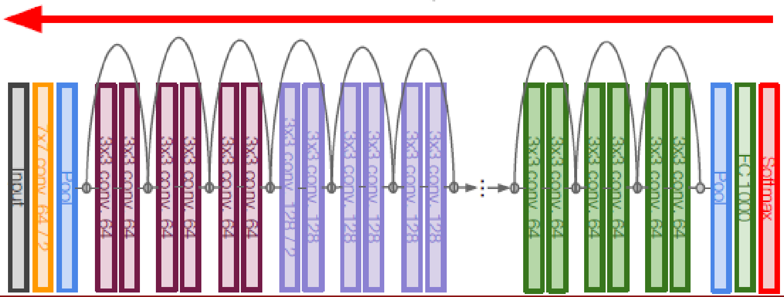
All internal vectors within GRU green frame have same length.
All ops within a purple circle are performed per element-wise on the ingoing vectors

Long Short Term Memory (LSTM): Gradient Flow

LSTM has an additional cell state C for a “long term memory”.



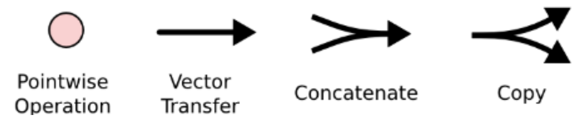
Similar to ResNet!



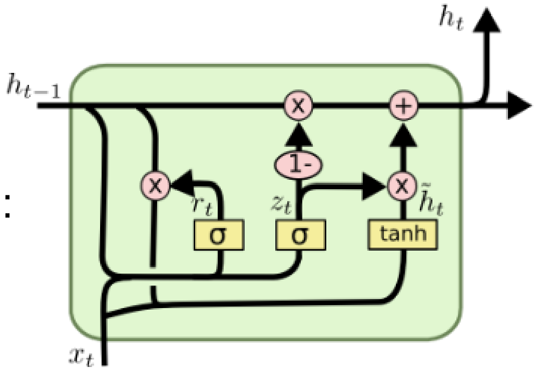
Long Short Term Memory networks (LSTM) were introduced by [Hochreiter & Schmidhuber (1997).]

Slide credit (modified): cs231 2017 stanford

Long Short Term Memory cell (LSTM) as GRU-extension

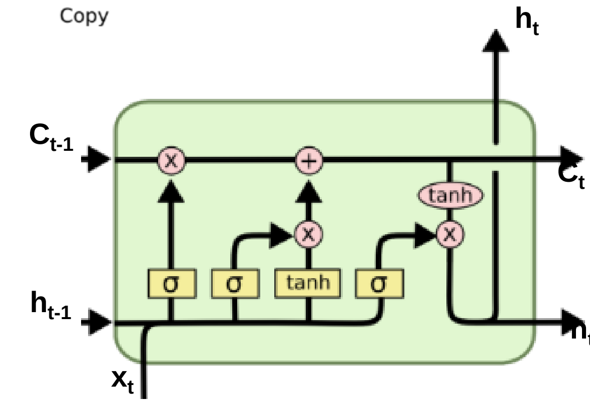


GRU-Cell:



$\mathbf{h}_t$

LSTM-Cell:



2 gates, 1 cell states (h)

Relevant gate: $\mathbf{r}_t = \sigma\left([\mathbf{h}_{t-1}, \mathbf{x}_t] \cdot \mathbf{W}_r + \mathbf{b}_r\right)$

Update gate: $\mathbf{z}_t = \sigma\left([\mathbf{h}_{t-1}, \mathbf{x}_t] \cdot \mathbf{W}_z + \mathbf{b}_z\right)$

Proposed hidden state: $\tilde{\mathbf{h}}_t = \tanh\left(\mathbf{x}_t \cdot \mathbf{W}_h + \mathbf{b}_h + \mathbf{h}_{t-1} \mathbf{U}_h \otimes \mathbf{r}_t\right)$

New hidden state is: $\mathbf{h}_t = (\mathbf{1}\text{-}\mathbf{z}_t) \otimes \tilde{\mathbf{h}}_t \oplus \mathbf{z}_t \otimes \mathbf{h}_{t-1}$

3 gates, 2 cell states (S:h, L:C)

Forget gate: $\mathbf{f}_t = \sigma\left([\mathbf{h}_{t-1}, \mathbf{x}_t] \cdot \mathbf{W}_f + \mathbf{b}_f\right)$

Input gate: $\mathbf{i}_t = \sigma\left([\mathbf{h}_{t-1}, \mathbf{x}_t] \cdot \mathbf{W}_i + \mathbf{b}_i\right)$

Output gate: $\mathbf{o}_t = \sigma\left([\mathbf{h}_{t-1}, \mathbf{x}_t] \cdot \mathbf{W}_o + \mathbf{b}_o\right)$

Proposed cell state: $\tilde{\mathbf{C}}_t = \tanh\left([\mathbf{h}_{t-1}, \mathbf{x}_t] \cdot \mathbf{W}_C + \mathbf{b}_C\right)$

New L cell state: $\mathbf{C}_t = \mathbf{f}_t \otimes \mathbf{C}_{t-1} \oplus \mathbf{i}_t \otimes \tilde{\mathbf{C}}_t$

New S hidden state: $\mathbf{h}_t = \mathbf{o}_t \otimes \tanh\left(\mathbf{C}_t\right)$

Credits: Colah blog http://colah.github.io/posts/2015-08-Understanding-LSTMs
LSTM: A Search Space Odyssey https://arxiv.org/abs/1503.04069 “all variants of LSTM achieved comparable performance”
An Empirical Exploration of Recurrent Network Architectures, Jozefowicz et al., 2015 10k RNN architectures – few outperformed lstm on few tasks

Long Short Term Memory (LSTM) in keras

dimension of vocabulary

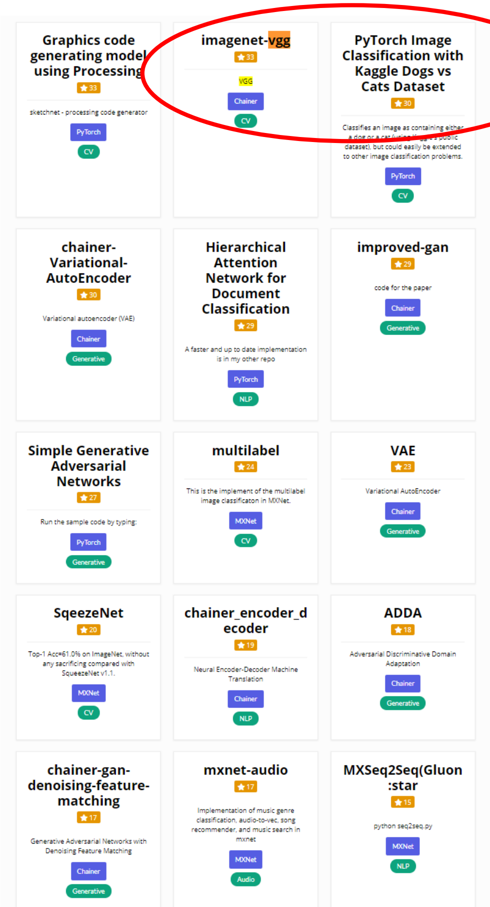
dimension of embedding

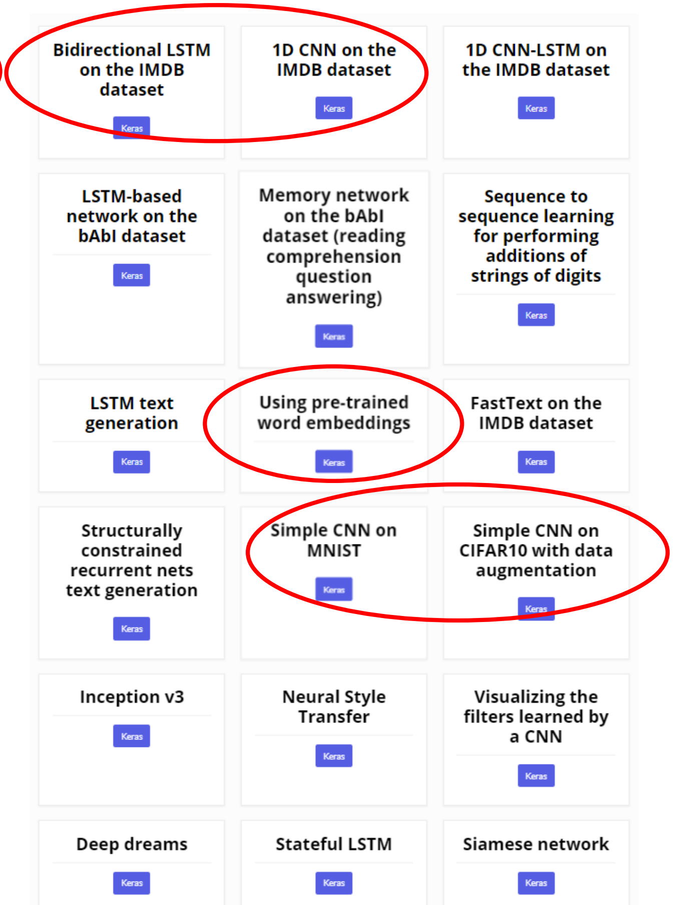
```
from keras.layers import LSTM

model = Sequential()
model.add(Embedding(max_features, 32))
model.add(LSTM(32))
model.add(Dense(1, activation='sigmoid'))

model.compile(optimizer='rmsprop',
              loss='binary_crossentropy',
              metrics=['acc'])
history = model.fit(input_train, y_train,
                    epochs=10,
                    batch_size=128,
                    validation_split=0.2)
```

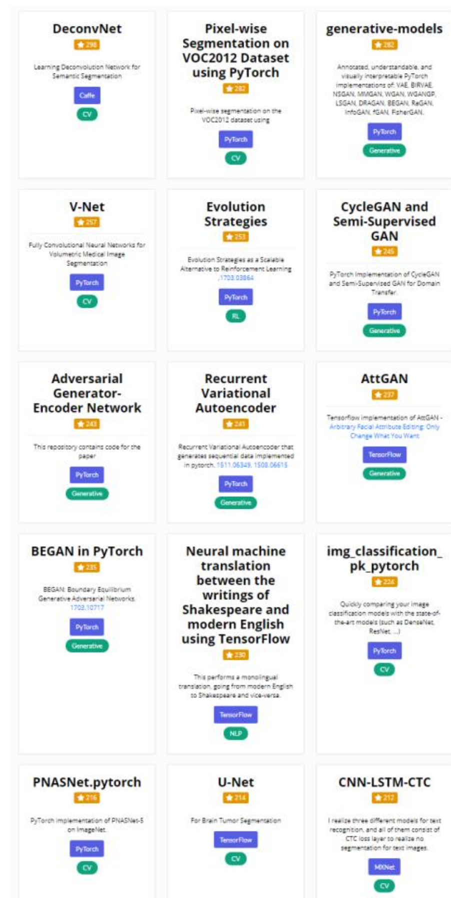
Model zoo: many pretrained NN are out there

https://modelzoo.co/

Base pretrained models and datasets in pytorch (MNIST, SVHN, CIFAR10, CIFAR100, STL10, AlexNet, VGG16, VGG19, ResNet, Inception, SqueezeNet)

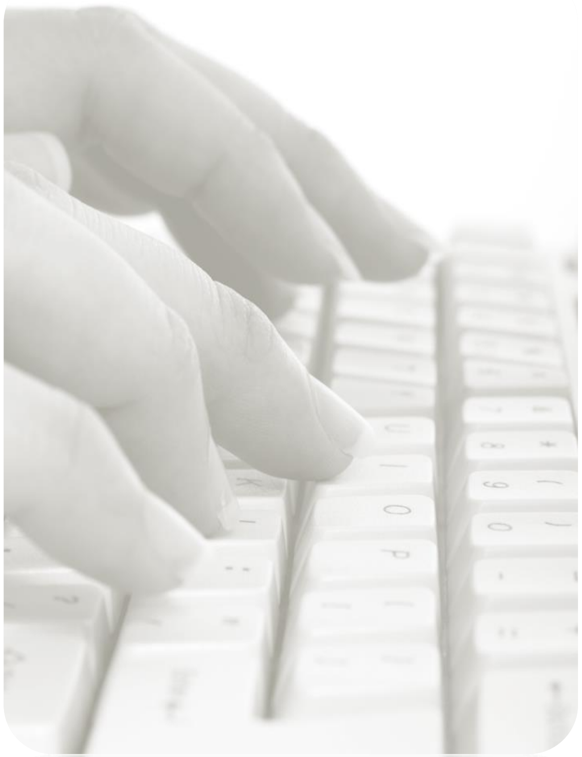






Can LSTM improve your conv1D series predictions?

- Work through the instructions in the second exercise in day 6 using https://github.com/tensorchiefs/dl_course_2018/blob/master/notebooks/12_LSTM_vs_1DConv.ipynb

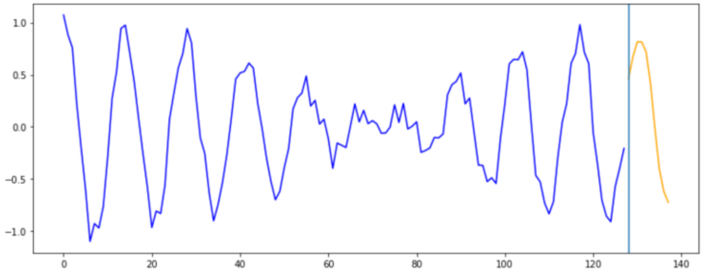


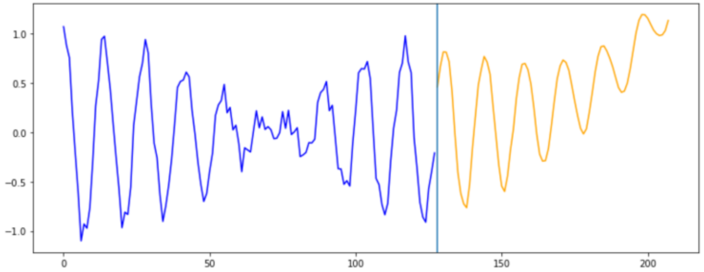
Exercise: predictions with numeric time-series

a) Open the notebook LSTM_vs_1DConv
Look at the data generating process and train the first "1D Convolution without dilation rate" model and look at the predictions for the next 10 and 80 time steps.
What to you observe, did the model learn the data generating process?
How big is the receptive field in the last convolutional layer?

```
model_1Dconv = Sequential()
ks = 5
model_1Dconv.add(Convolution1D(filters=32, kernel_size=ks, padding='causal', input_shape=(128, 1)))
model_1Dconv.add(Convolution1D(filters=32, kernel_size=ks, padding='causal'))
model_1Dconv.add(Convolution1D(filters=32, kernel_size=ks, padding='causal'))
model_1Dconv.add(Convolution1D(filters=32, kernel_size=ks, padding='causal'))
model_1Dconv.add(Dense(1))
model_1Dconv.add(Lambda(slice, arguments={'slice_length':look_ahead}))

model_1Dconv.compile(optimizer='adam', loss='mean_squared_error')
model_1Dconv.summary()
```

$$ReceptiveField = f_0 \cdot d_0 + \sum_i (f_i - 1) \cdot d_i$$
$$= 5 \cdot 1 + 4 \cdot 1 + 4 \cdot 1 + 4 \cdot 1 = 17$$





Exercise: predictions with numeric time-series

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Look at the data generating process and train the first “1D Convolution without dilation rate” model and look at the predictions for the next 10 and 80 time steps.
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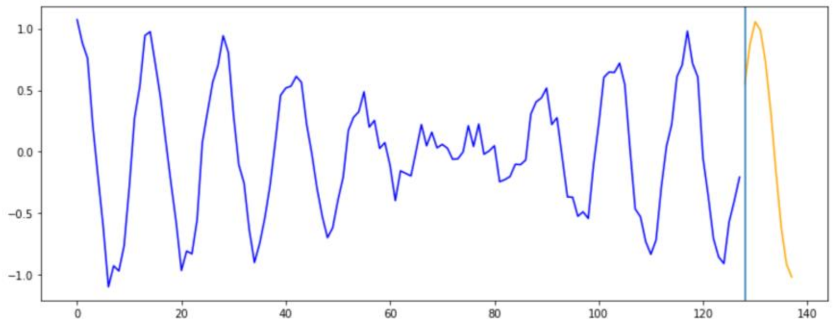
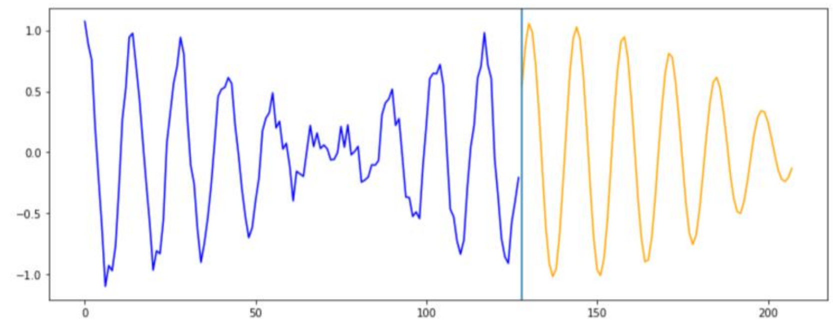
How big is the receptive field in the last convolutional layer?

```
model_1Dconv_w_d = Sequential()
ks = 5
model_1Dconv_w_d.add(Convolution1D(filters=32, kernel_size=ks, padding='causal', dilation_rate=1, input_sh
ape=(128, 1)))
model_1Dconv_w_d.add(Convolution1D(filters=32, kernel_size=ks, padding='causal', dilation_rate=2))
model_1Dconv_w_d.add(Convolution1D(filters=32, kernel_size=ks, padding='causal', dilation_rate=4))
model_1Dconv_w_d.add(Convolution1D(filters=32, kernel_size=ks, padding='causal', dilation_rate=8))
model_1Dconv_w_d.add(Dense(1))
model_1Dconv_w_d.add(Lambda(slice, arguments={'slice_length':look_ahead}))

model_1Dconv_w_d.compile(optimizer='adam', loss='mean_squared_error')
model_1Dconv_w_d.summary()
```

$$ReceptiveField = f_0 \cdot d_0 + \sum_i (f_i - 1) \cdot d_i$$

$$= 5 \cdot 1 + 4 \cdot 2 + 4 \cdot 4 + 4 \cdot 8 = 61$$





Exercise: perditions with numeric time-series

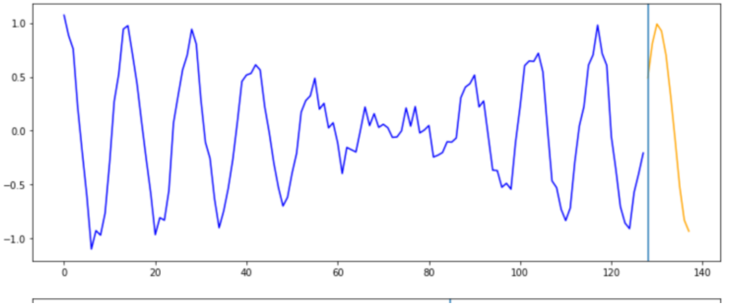
c) Now, Let's use a RNN for the same process. How good are the predictions for the 10 and 80 time steps?
What does the argument return_sequences mean?
How many weights do we need if we use a hidden state size of 12, check your calculations with the model.summary().
Did the model learn the data generating process?

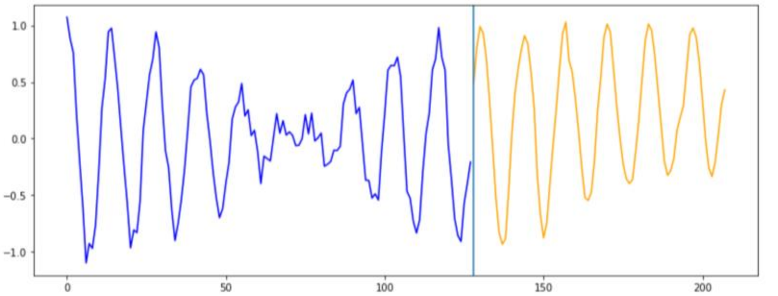
```
model_simple_RNN = Sequential()

model_simple_RNN.add(SimpleRNN(12,return_sequences=True,input_shape=(128,1)))
model_simple_RNN.add((Dense(1)))
model_simple_RNN.add(Lambda(slice, arguments={'slice_length':look_ahead}))

model_simple_RNN.summary()
model_simple_RNN.compile(optimizer='adam', loss='mean_squared_error')
```

```
_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
simple_rnn_1 (SimpleRNN)     (None, 128, 12)           168
_________________________________________________________________
dense_3 (Dense)              (None, 128, 1)            13
_________________________________________________________________
lambda_3 (Lambda)            (None, 10, 1)             0
=================================================================
Total params: 181
Trainable params: 181
Non-trainable params: 0
```

Von (12+1) auf 12: (12+1)*12+12=168

Von (12) auf 1: (12)*1+1=13





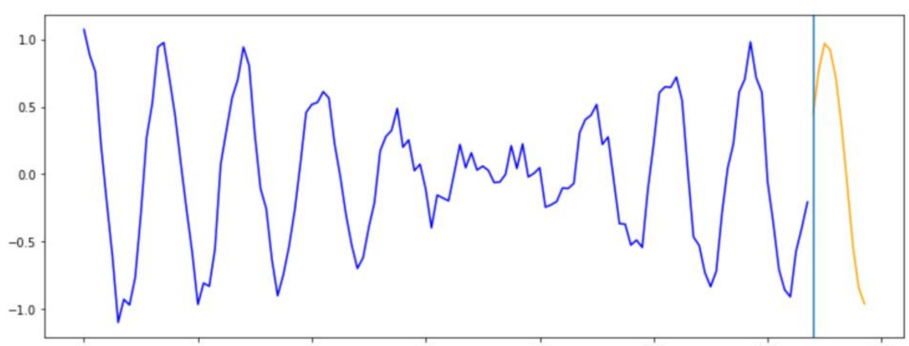
Exercise: predictions with numeric time-series

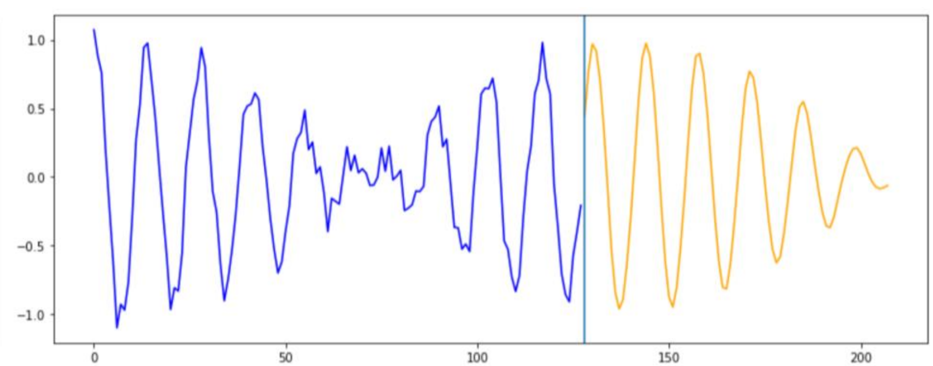
d) Let's replace the RNN cell with a more complex LSTM cell, in keras LSTM.
Use the same size of units and the same architecture.
How many weights do we need now?

```
model_LSTM = Sequential()

model_LSTM.add(LSTM(12,return_sequences=True,input_shape=(128,1)))
model_LSTM.add((Dense(1)))
model_LSTM.add(Lambda(slice, arguments={'slice_length':look_ahead}))

model_LSTM.summary()
model_LSTM.compile(optimizer='adam', loss='mean_squared_error')
```

```
_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
lstm_1 (LSTM)                (None, 128, 12)           672
_________________________________________________________________
dense_4 (Dense)              (None, 128, 1)            13
_________________________________________________________________
lambda_4 (Lambda)            (None, 10, 1)             0
=================================================================
Total params: 685
Trainable params: 685
Non-trainable params: 0
_________________________________________________________________
```

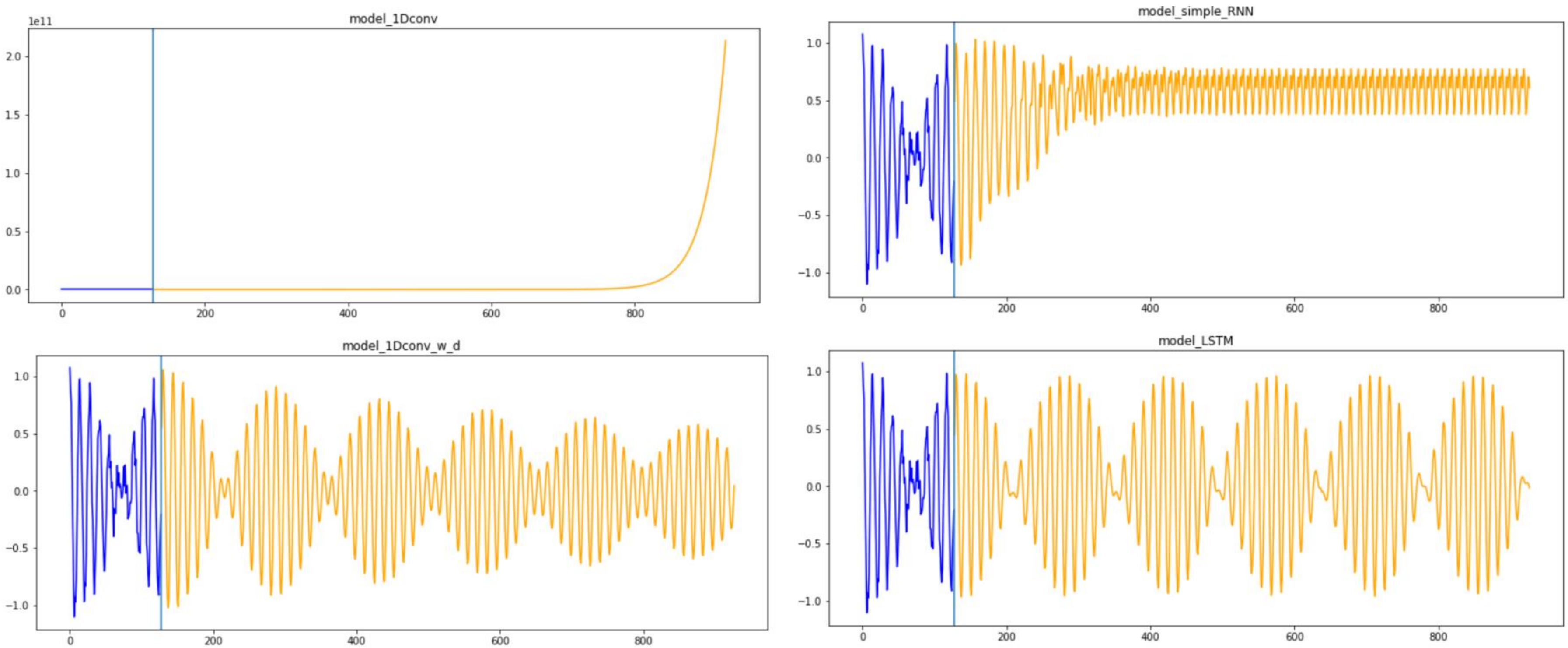
We have 4 –times from (h,x) to h
Here (12+1) to 12:
4*((12)*13+12)=672





Exercise: predictions with numeric time-series

e) Compare the 4 models for very long predictions (800 timesteps). What do you observe? What could we do to improve the RNN and the Conv1D with dilation_rate?



To improve the performance, we would try to enlarge the memory and allow for more flexible models:
1D-CNN: stack more dilated layers to get a receptive field that sees whole input
RNN, LSTM: enlarge the dimension of the hidden state and stack more layers.

Time for your project