PROBABILISTIC AND DIFFERENTIABLE PROGRAMMING

V4: Deep Learning II (RNNs and Reservoir)

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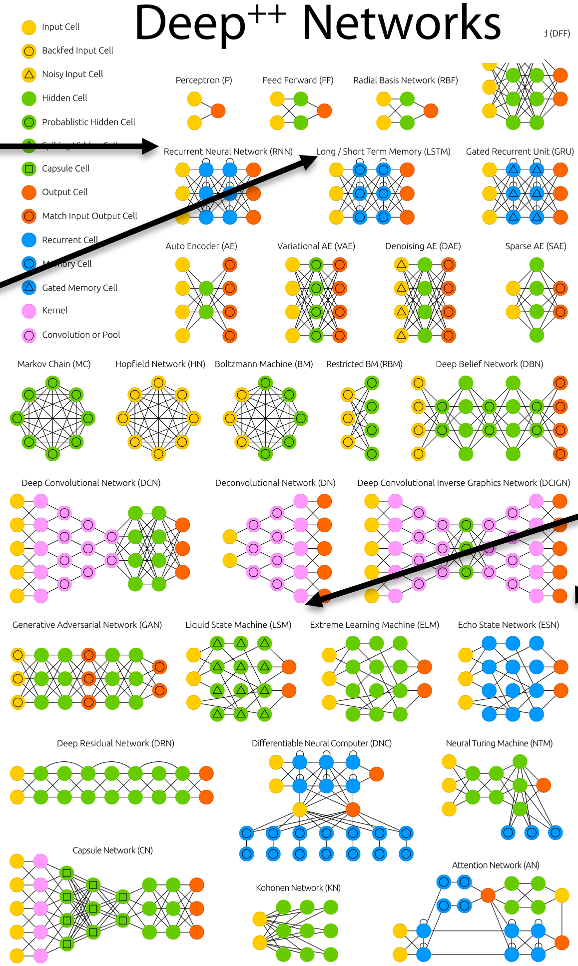
Today‘s Agenda

1. Follow me:
Recurrent networks

2. Some things to remember, some things to forget:
Long short term memory

Deep^{++} Networks



3. Forget to learn the hiddens:
Reservoir Computing

Example Named Entity recognition

x_1 x_2 x_3 x_4 x_5 x_6 x_7

- **x**: Jon and Ethan gave deep learning lectures

- **y**: 1 0 1 0 0 0 0

y_1 y_2 y_3 y_4 y_5 y_6 y_7

- In this case input and output vector of length 7
- But naturally longer sequences are possible

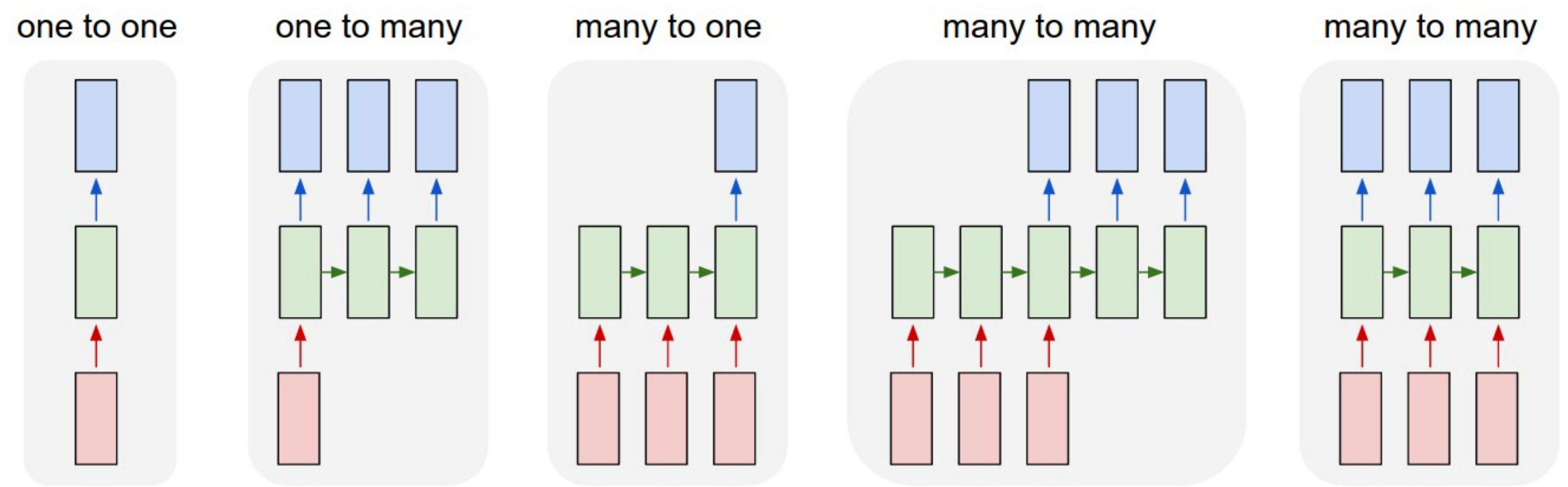


Image classification
In: image
Out: Classifier

Image captioning
In: image
Out: sentence

Sentimental analysis
In: sentence
Out: sentiment

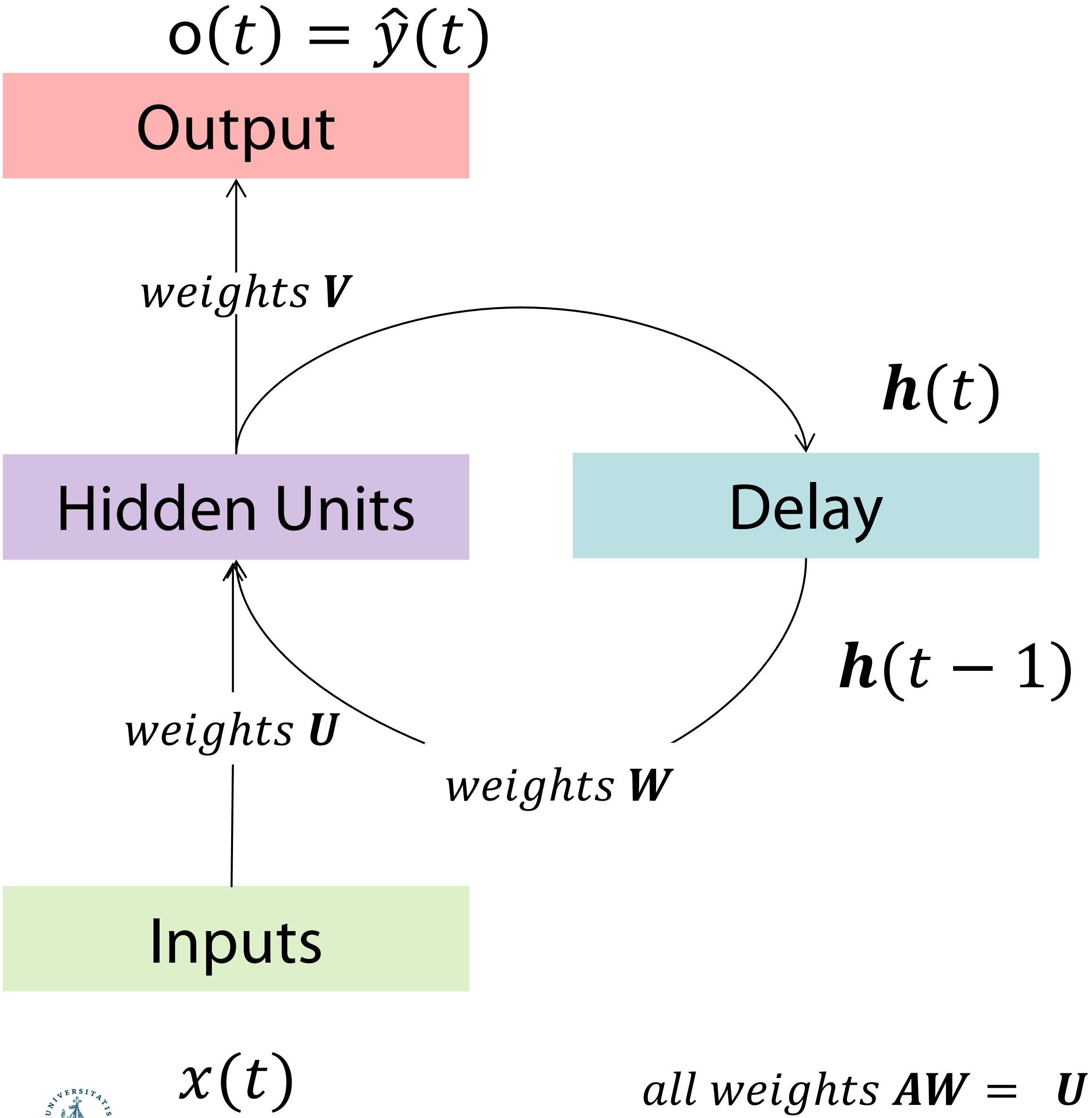
Machine translation
In: sentence
Out: sentence

Synced video
In: video
Out: real-time labels

Why Not a Standard Feed Forward Network?

- For a task such as "Named Entity Recognition" a MLP (multi-layer perceptron) would have several disadvantages
  - The inputs and outputs may have varying lengths
  - The features wouldn't be shared across different temporal positions in the network
    - Note that 1-D convolutions can be (and are) used to address this, in addition to RNNs
- To interpret a sentence or to predict tomorrows weather it is necessary to remember what happened in the past
- To facilitate this we would like to add a feedback loop delayed in time

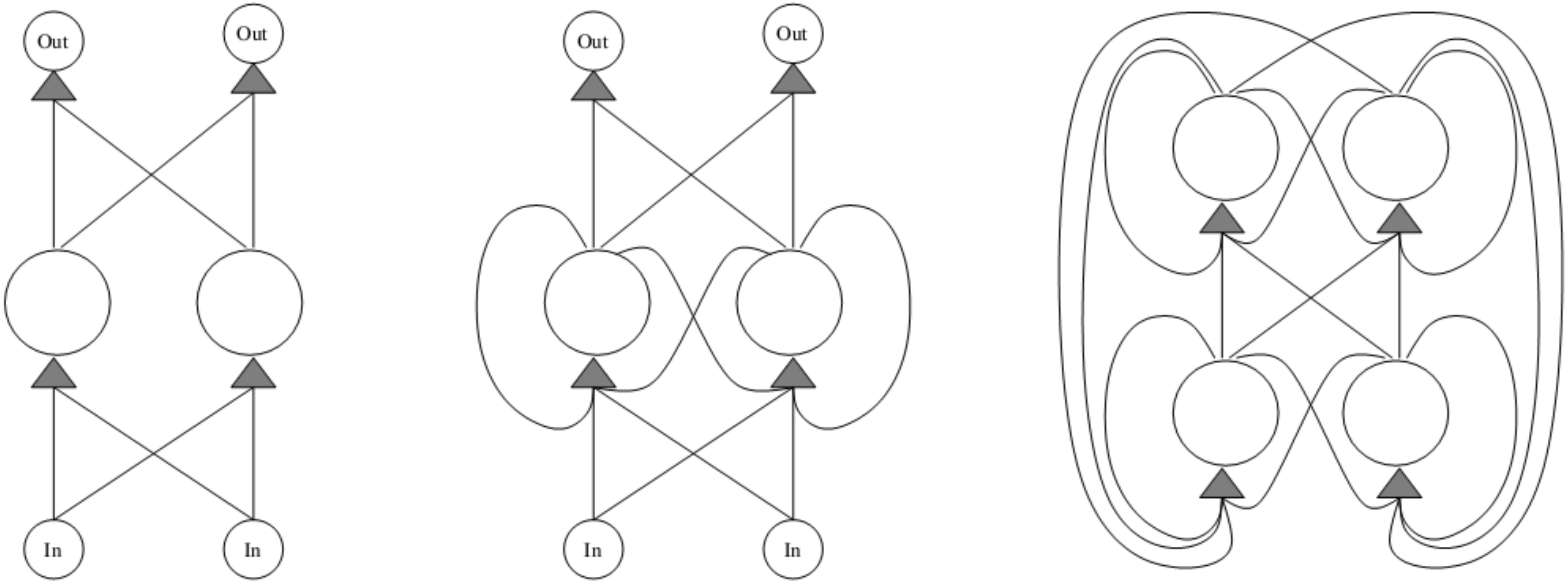
RNN Architecture



- RNNs are NNs for processing sequential data
- Contain directed cycles in their computational graph
  - Another form of „more structure“ in DL
  - Another form of parameter sharing in DL

$$all\ weights\ \boldsymbol{AW} = \boldsymbol{U} \cup \boldsymbol{V} \cup \boldsymbol{W}$$

RNN Architecture



Left: feed forward neural network
Middle: a simple recurrent neural network
Right: Fully connected recurrent neural network

An RNN is just a recursive function invocation

- Output update

$$\hat{\boldsymbol{y}}\,(t) = \boldsymbol{f_o}(\boldsymbol{x}\,(t), \boldsymbol{h}(t\,-\,1)|\boldsymbol{AW}\,)$$

- State update

$$\boldsymbol{h}(t)\; = \boldsymbol{f_h}(\boldsymbol{x}\,(t), \boldsymbol{h}(t\,-\,1)|\boldsymbol{AW}\,)$$

- If $\hat{\boldsymbol{y}}(t)$ depends on the input $\boldsymbol{x}(t\,-\,2)$, then prediction will be $\boldsymbol{f_o}\,(\boldsymbol{x}\,(t), \boldsymbol{f_h}(\boldsymbol{x}\,(t\,-\,1), \boldsymbol{f_h}(x\,(t\,-\,2), \boldsymbol{f_h}(x\,(t-\,3)|\boldsymbol{AW}\,)|\boldsymbol{AW}\,)|\boldsymbol{AW}\,)|\boldsymbol{AW}\,)$
- Gradients of this with respect to the weights can be found with the chain rule

Variants of RNNs

- Depending on the instantiation of $\boldsymbol{f_h}()$
  - Elman (Vanilla/Simple Networks)
  - Jordan (not discussed here)
  - LSTM (discussed here)
  - GRU (Gated recurrent unit; not discussed here)

  - Elman
    - $\boldsymbol{h}_t = \boldsymbol{f_h}(\boldsymbol{U}\boldsymbol{x}_t + \boldsymbol{b_U} + \boldsymbol{W}\boldsymbol{h}_{t-1} + \boldsymbol{b_W}) = \boldsymbol{f_h}(\boldsymbol{a_h}(t))$
    - $\hat{\boldsymbol{y}}_t = \boldsymbol{o}(t) = f_o(\boldsymbol{V}h_t + \boldsymbol{b_o}) = \boldsymbol{f_o}(\boldsymbol{a_o}(t))$
    - $\boldsymbol{f_h}$ is usally $tanh$
    - $\boldsymbol{f_o}$ identity or logit

RNNs combine two properties which make them very powerful.

1. Distributed hidden state that allows them to store a lot of information about the past efficiently. This is because several different units can be active at once, allowing them to remember several things at once.
2. Non-linear dynamics that allows them to update their hidden state in complicated ways.

- In particular: RNNs are universal approximators

Going Deep with RNNs

- You can go deep w.r.t. time unfolding (some do not consider this as going deep)
- As RNNs calculate functions, you can compose them (stack the RNNs)

  $$\hat{\boldsymbol{y}}\,(t) = \boldsymbol{f_o^2}\,(\boldsymbol{f_o^1}\,(\boldsymbol{x}\,(t\,), \boldsymbol{h^1}(t-1)|\boldsymbol{AW_1}\,), \boldsymbol{h^2}(t-1)|\boldsymbol{AW_2}\,)$$

  – The output of the inner RNN at time t is fed into the input of the outer RNN which produces the prediction $\hat{\boldsymbol{y}}$
- You could of course also add feedfoward parts into the input block or the output block or the hidden block

Example: Character-level language modelling

- An RNN that learns to 'generate' English text by learning to predict the next character in a sequence
- This is "Character-level Language Modelling"

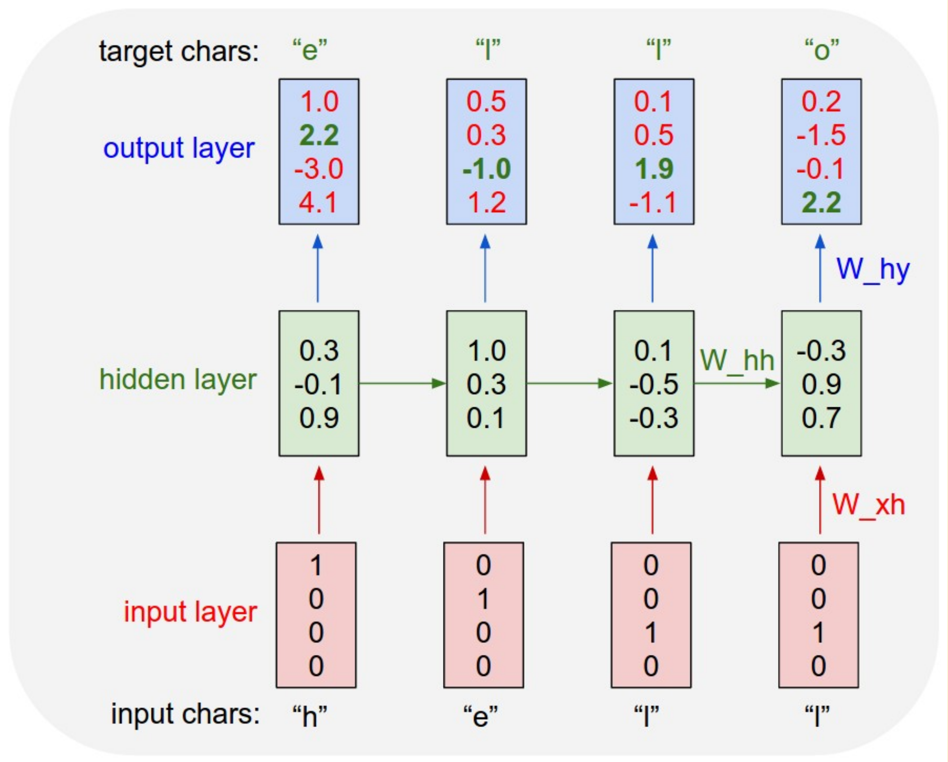


Image from http://karpathy.github.io/2015/05/21/rnn-effectiveness/

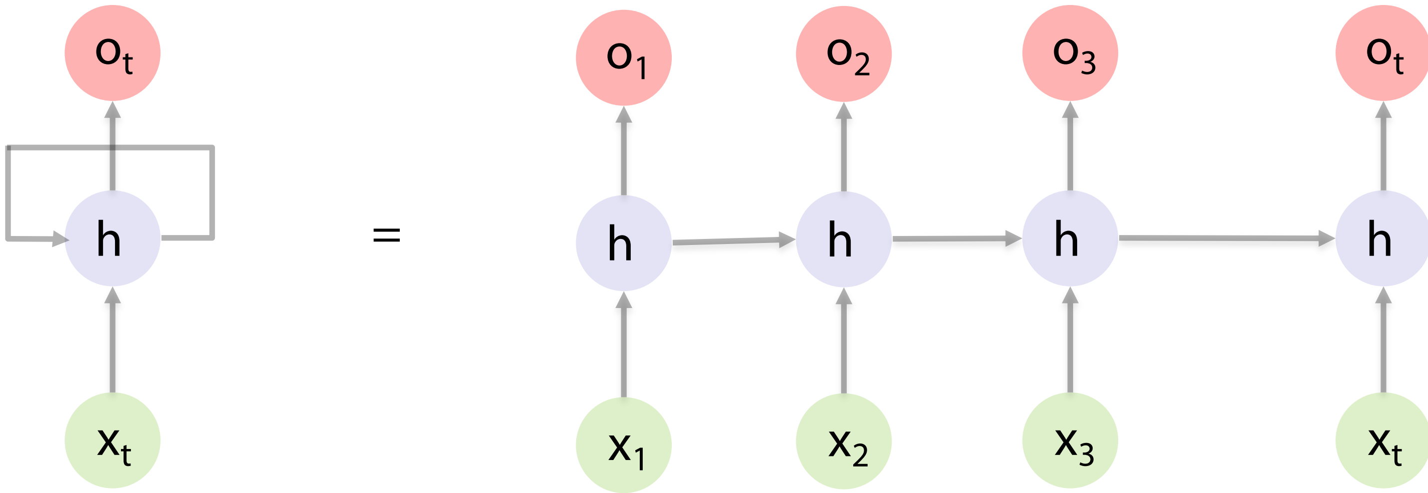
Training and sampling the Language Model

- The training data is just text data (e.g. sequences of characters)
- The task is unsupervised (or rather self-supervised): given the previous characters predict the next one
- All you need to do is train on a reasonable sized corpus of text
- Overfitting could be a problem: dropout is very useful here

- Once the model is trained can generate text
  - See examples at http://karpathy.github.io/2015/05/21/rnn-effectiveness/

Recurrent Neural Neworks unfolded

- Can unravel/unfold network into feed forward
  - can apply gradient descent/timed backpropagation (BPTT: Backpropagation through time)
  - Minimize error $\sum_t ||y(t) - \hat{y}(t)||^2$ over all time steps



Back Propagation Through Time (BPTT)

- BPTT learning algorithm is an extension of standard backpropagation that performs gradients descent on an unfolded network.

- The gradient descent weight updates have contributions from each time step.

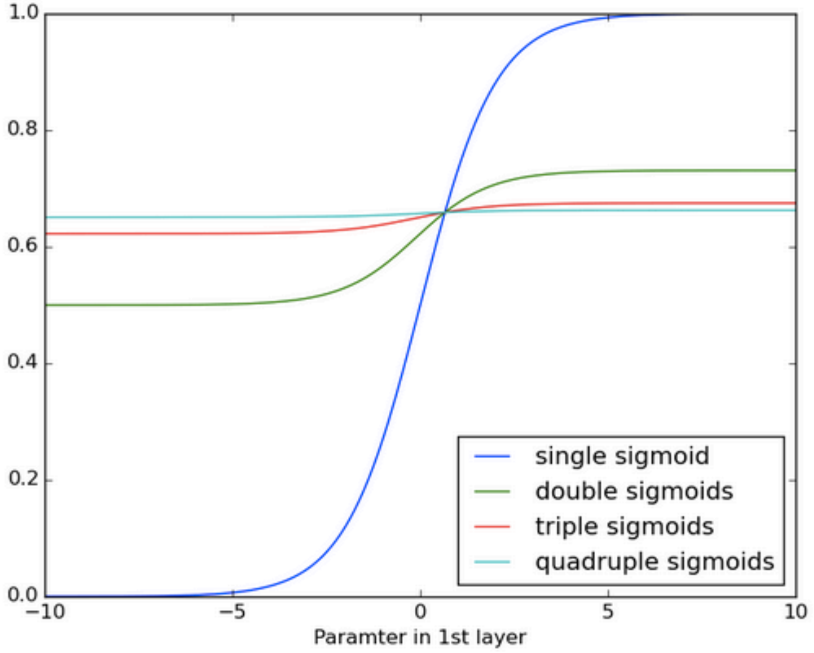
- The errors have to be back-propagated through time as well as through the network

RNN Backward Pass

- Loss function depends on the activation of the hidden layer through its influence on the output layer **and** through its influence on the hidden layer at the next step.
  - $h_t = f_h(x, h_{t-1}, W)$
  - $o_t = f_o(h_t, V)$
- The interesting part is the calculation of the gradient w.r.t. the hidden parameters W
  - $E = \sum_{t=1}^{T} E_t$ (error in RNN)
  - $\frac{\partial E}{\partial W} = \sum_{t=1}^{T} \frac{\partial E_t}{\partial W} = \sum_{t=1}^{T} \frac{\partial E_t}{\partial o_t} \frac{\partial o_t}{\partial h_t} \frac{\partial h_t}{\partial W}$
  - $\frac{\partial h_t}{\partial W} = \frac{\partial f_h(x_t, h_{t-1}, W)}{\partial W} + \frac{\partial f_h(x_t, h_{t-1}, W)}{\partial h_{t-1}} \frac{\partial h_{t-1}}{\partial W}$ (by chain rule)
  - $\frac{\partial h_t}{\partial W} = \frac{\partial f_h(x_t, h_{t-1}, W)}{\partial W} + \sum_{i=1}^{t-1} \left(\prod_{j=i+1}^{t} \frac{\partial h_j}{\partial h_{j-1}} \right) \frac{\partial f_h(x_i, h_{i-1}, W)}{\partial W}$

(by solving the recursion)

Here they come again: Vanishing and exploding Gradients



=>Solution: Long short term memory networks (LSTMs)

LONG SHORT TERM MEMORY

LSTM - introduction

- LSTM was invented to solve the vanishing gradients problem.
- LSTM maintain a more constant error flow in backprapogation.
  - Long term memory by specific hidden state c(t) = c(t-1)
  - Sometimes one has to forget and sometimes have to change the memory
  - To do this use gates saturating at 0 (read/write denied) and 1 (read/write allowed) => Sigmoid
- LSTM can handle global dependencies (1000 time steps)

LSTM Architecture

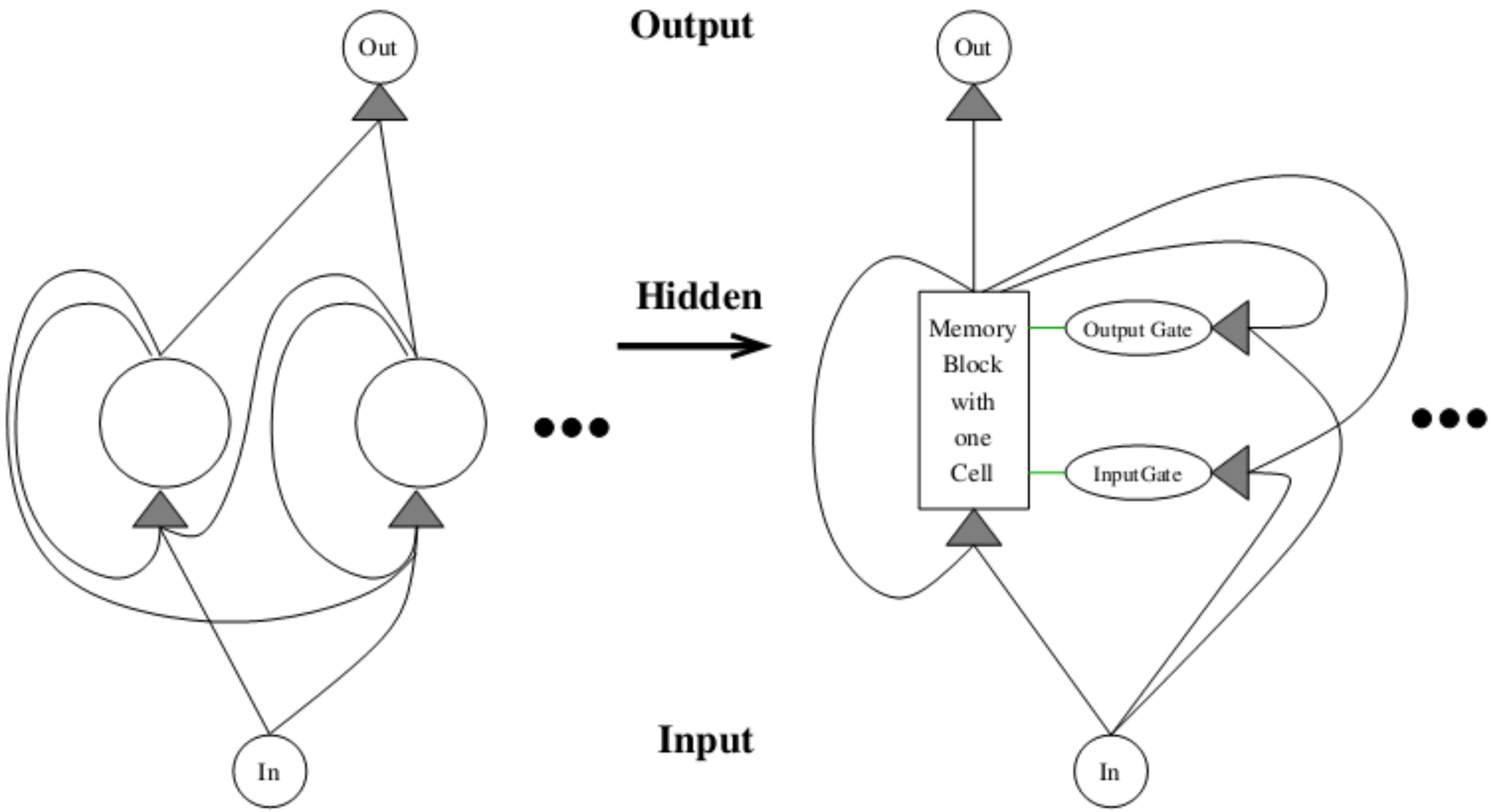
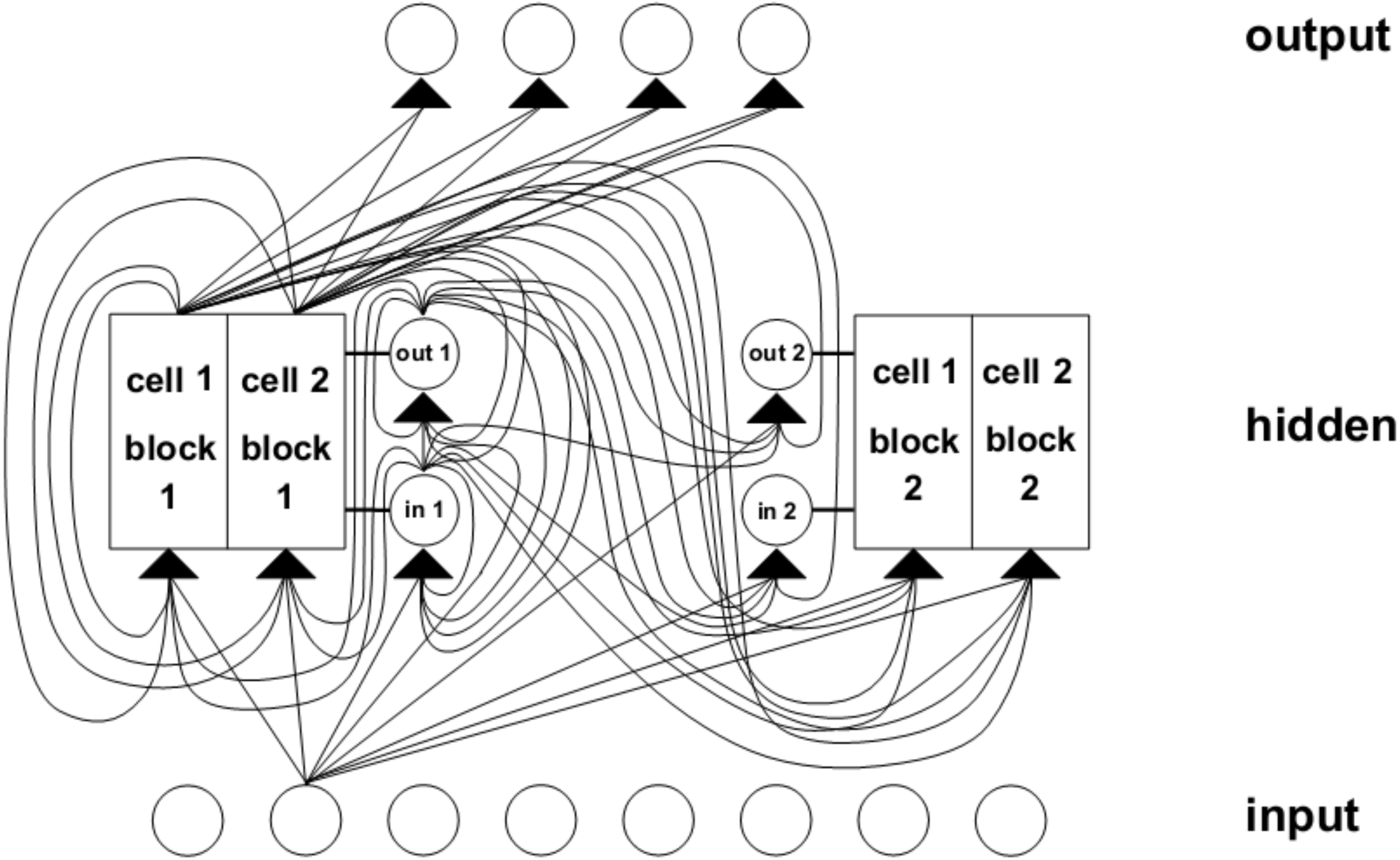
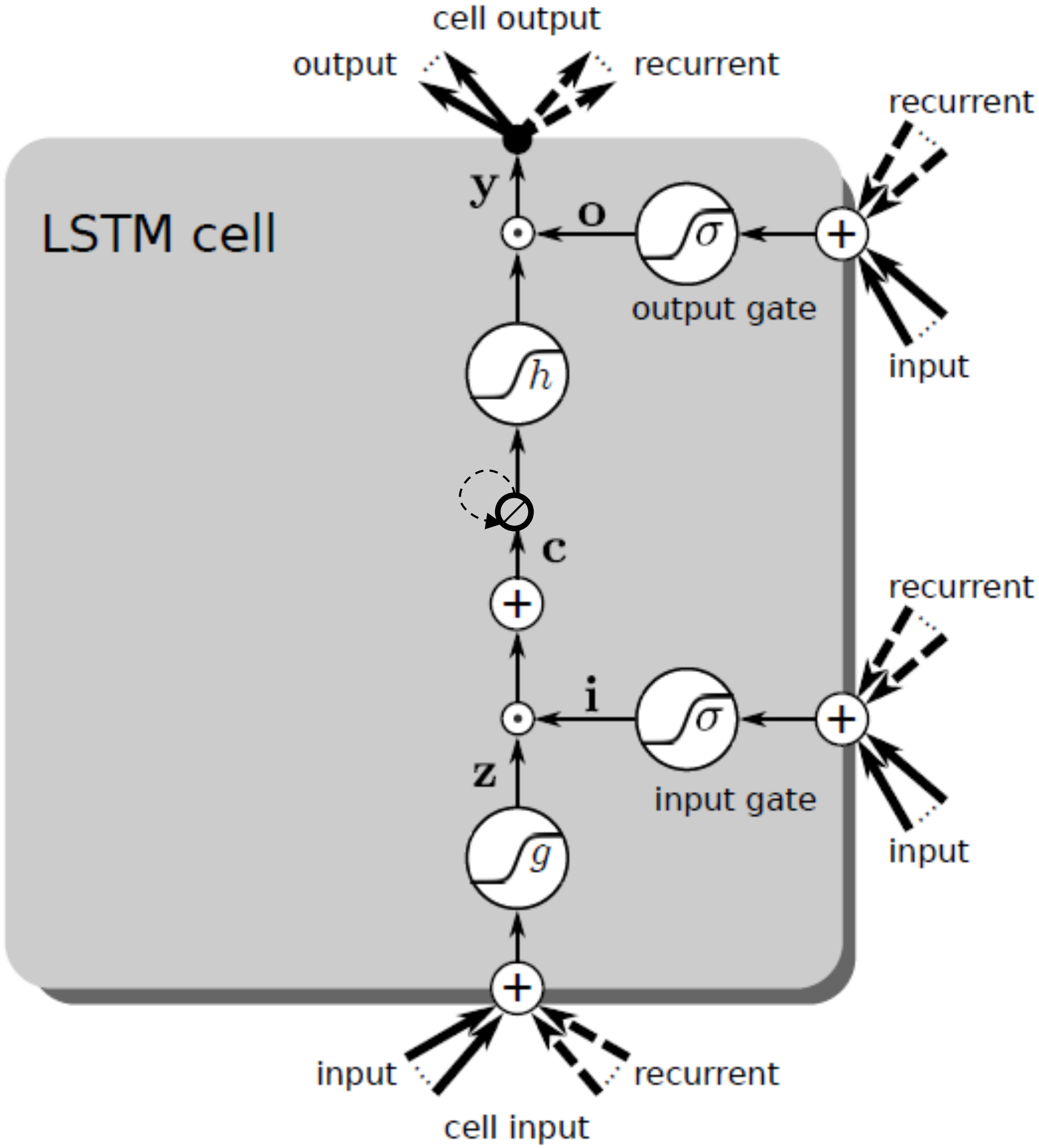


Figure 2.1: Left: RNN with one fully recurrent hidden layer. Right: LSTM network with memory blocks in the hidden layer (only one is shown).

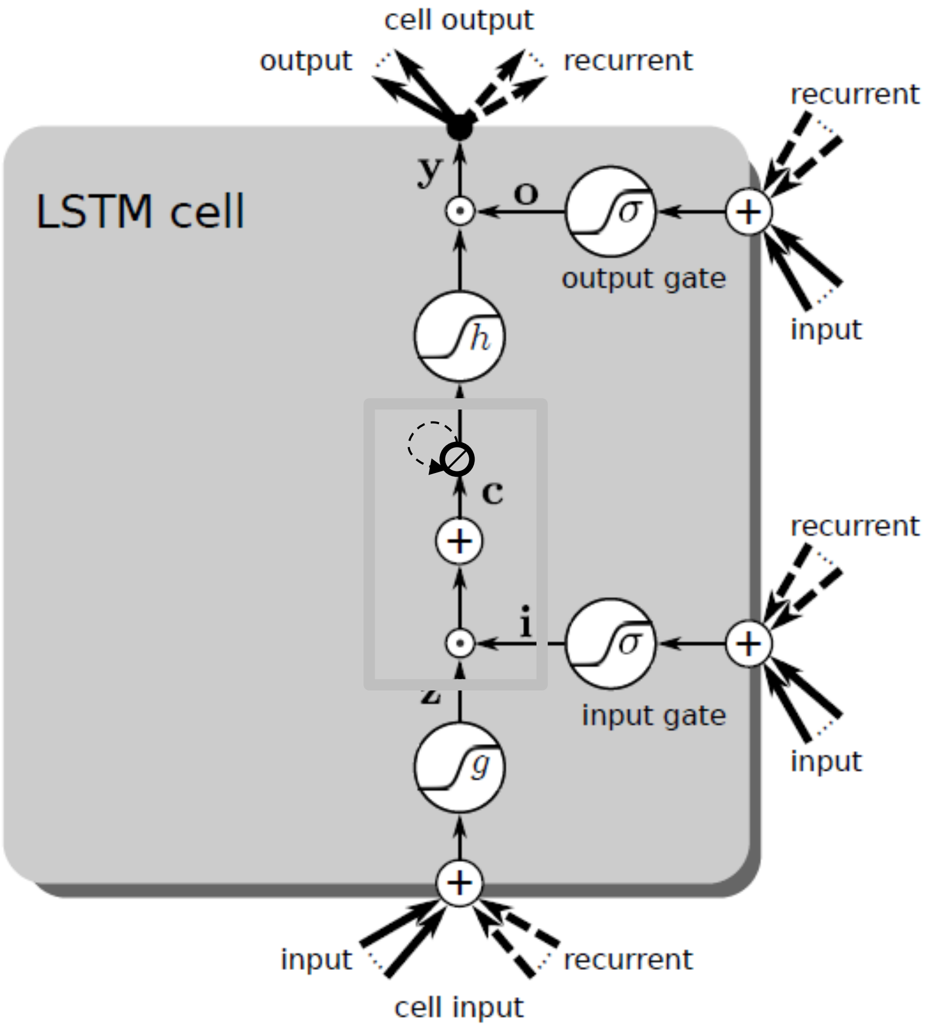
LSTM Architecture



LSTM Architecture - overview



LSTM Architecture – long term memory cell

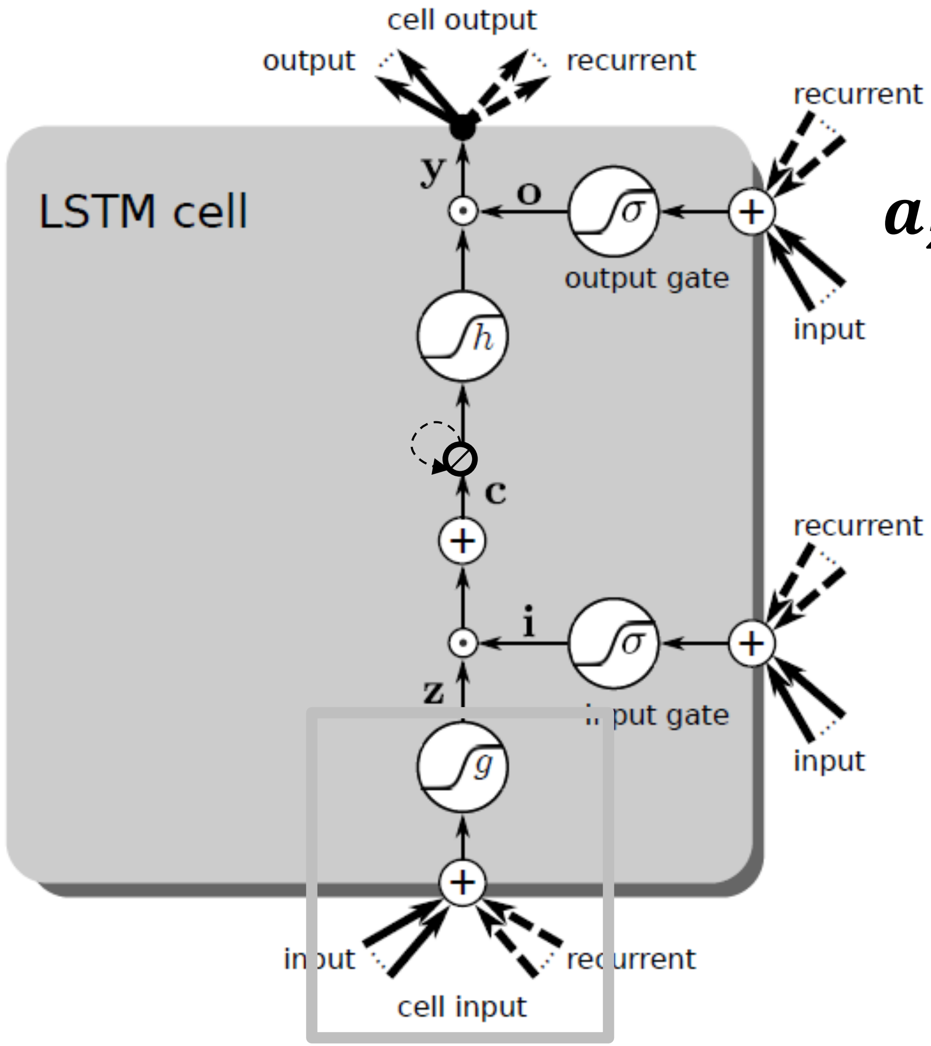


- Each memory cell contains a node with a self-connected recurrent edge of fixed weight one
- Ensures that the gradient can pass across many time steps without vanishing
- CEC (constant error carousel)

- => Long term memory
- In contrast: Previous outputs from hidden: short term memory

$$c(t) = z(t) \odot i(t) + c(t-1)$$

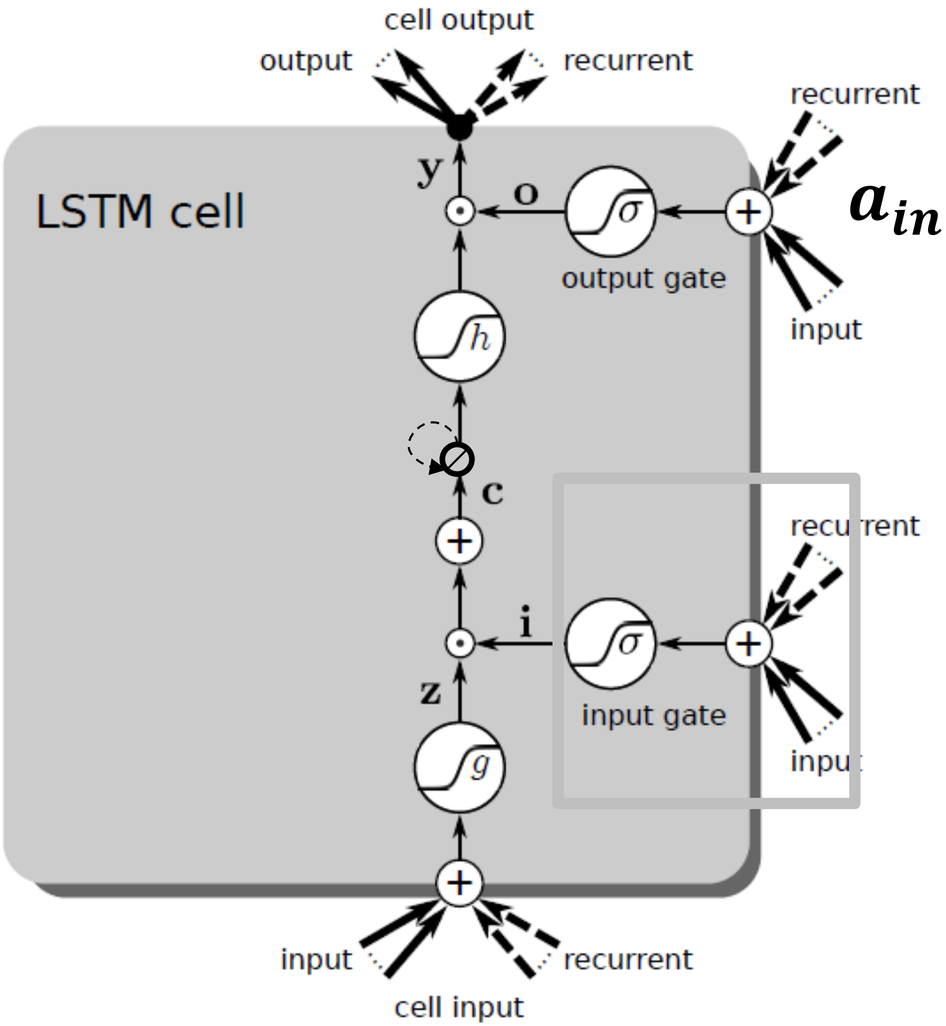
LSTM Architecture – input



$$\boldsymbol{a}_z(t) = \boldsymbol{W}_z\boldsymbol{x}(t) + \boldsymbol{R}_z\boldsymbol{y}(t-1)$$
$$z(t) = g\big(\boldsymbol{a}_z(t)\big)$$

(control forwarding of input and previous step information)

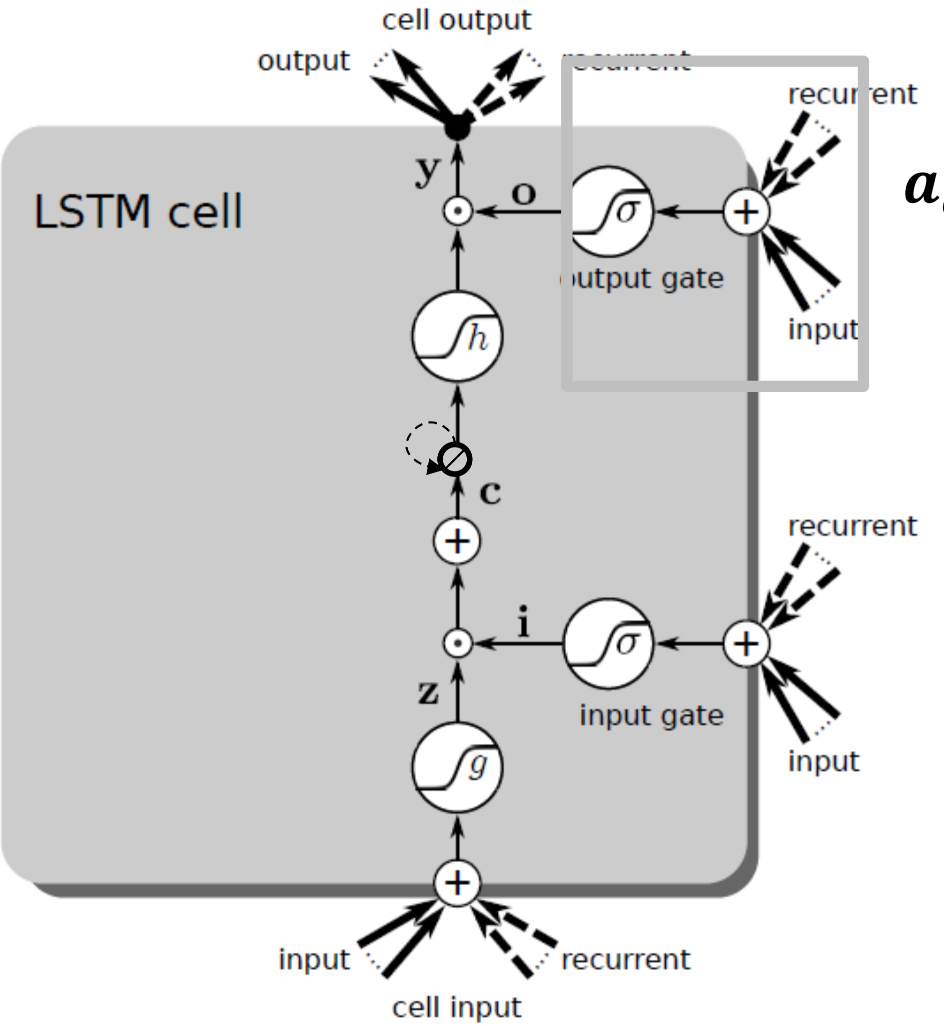
LSTM Architecture – input gate



$$a_{in}(t) = W_{in}x(t) + R_{in}y(t-1)$$
$$i(t) = \sigma\left(a_{in}(t)\right)$$

(control write access to memory cells)

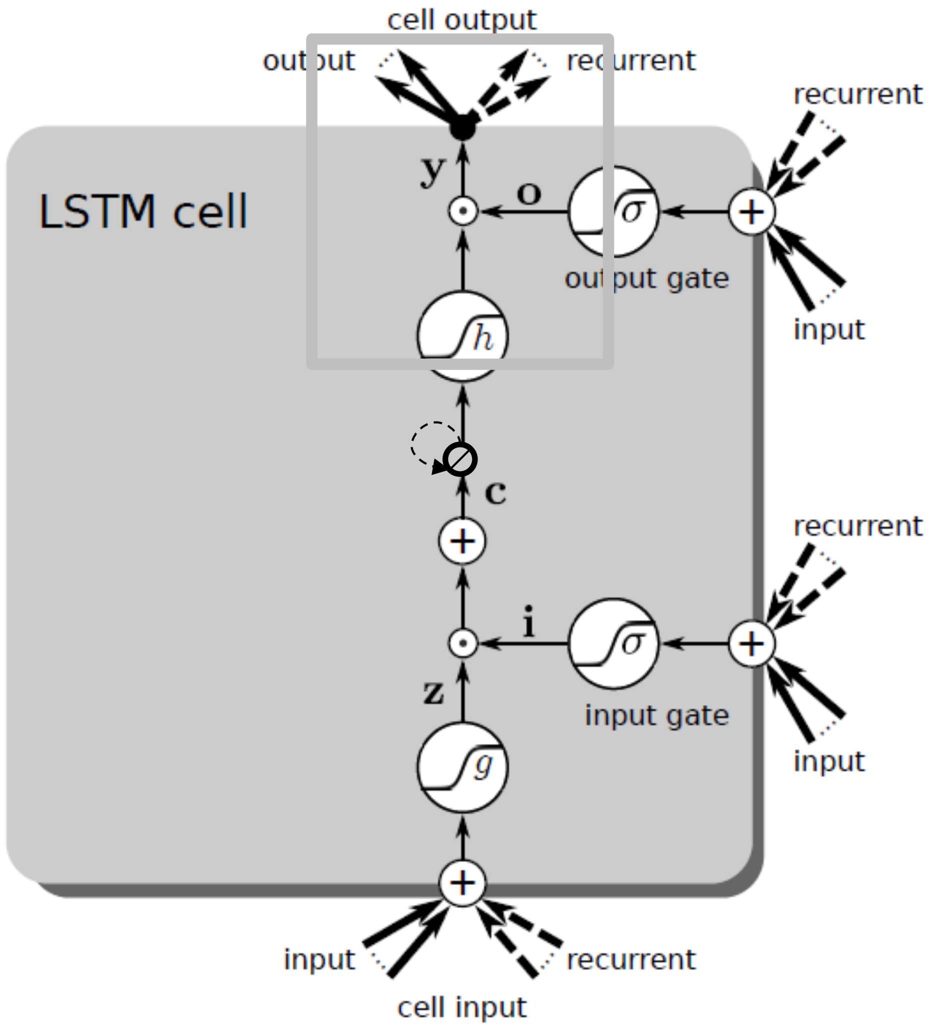
LSTM Architecture – Output gate



$$\boldsymbol{a}_{\boldsymbol{out}}(t) = \boldsymbol{W}_{\boldsymbol{out}}\boldsymbol{x}(t) + \boldsymbol{R}_{\boldsymbol{out}}\boldsymbol{y}(t-1)$$
$$o(t) = \sigma\big(\boldsymbol{a}_{\boldsymbol{out}}(t)\big)$$

(control read access to memory cell)

LSTM Architecture – Output gate



$$\boldsymbol{y}(t) = \boldsymbol{h}\big(\boldsymbol{c}(t)\big) \odot \boldsymbol{o}(t)$$

(control outputting of memory cell content via o(t))

LSTM Forward Pass

- The cell state c is updated based on its current state and 3 inputs: a_z , a_{in} , a_{out}

$$a_z(t) = W_z x(t) + R_z\big(y(t-1)\big)\,, z(t) = g\big(a_z(t)\big)$$

$$a_{in}(t) = W_{in} x(t) + R_{in}\big(y(t-1)\big)\,, i(t) = \sigma\big(a_{in}(t)\big)$$

$$c(t) = z(t) \odot i(t) + c(t-1)$$

$$a_{out}(t) = W_{out} x(t) + R_{out}\big(y(t-1)\big)\,, o(t) = \sigma\big(a_{out}(t)\big)$$

$$y(t) = h\big(c(t)\big) \odot o(t)$$

LSTM Backward Pass

- Errors arriving at cell outputs are propogated to the CEC
- Errors can stay for a long time inside the CEC
- This ensures non-decaying error
- Can bridge time lags between input events and target signals

- (details left out here)

An addition: Handling unbounded memory

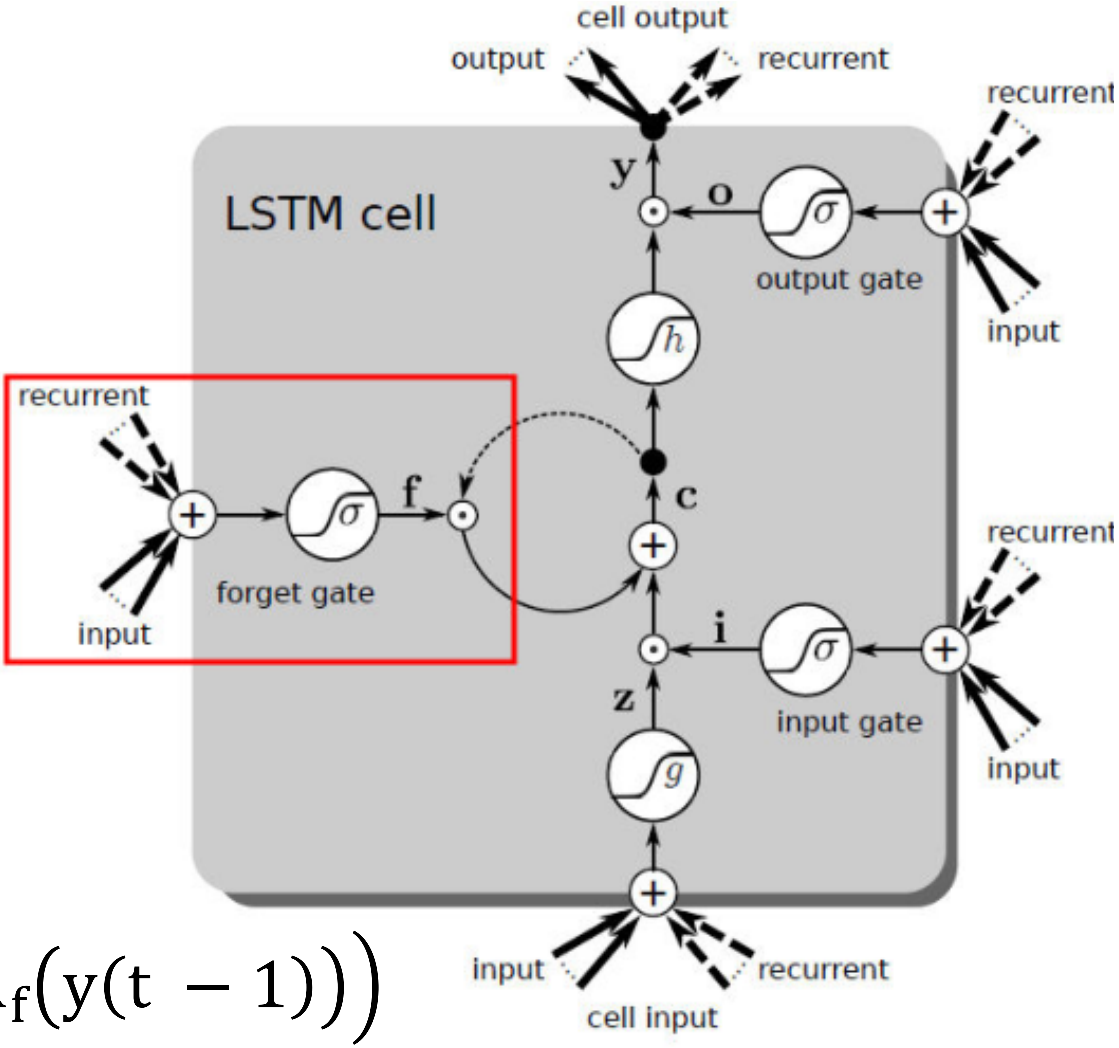
$c(t) = z(t) \odot i(t) + c(t-1) \rightarrow$ grows linearly

For a continuous input stream →
$c(t)$ may grow in an unbounded fashion →
can cause a saturation in $h(t)$

$$\delta_c(t) = \delta_y(t) h'\big(c(t)\big) \odot o(t)$$

Small gradients

LSTM possible remedy by forget gate



$$f(t) = \sigma\left(\mathrm{W_f x(t)} + \mathrm{R_f}\big(\mathrm{y(t} - 1)\big)\right)$$

$$c(t) = z(t) \odot i(t) + f(t) \odot c(t-1)$$

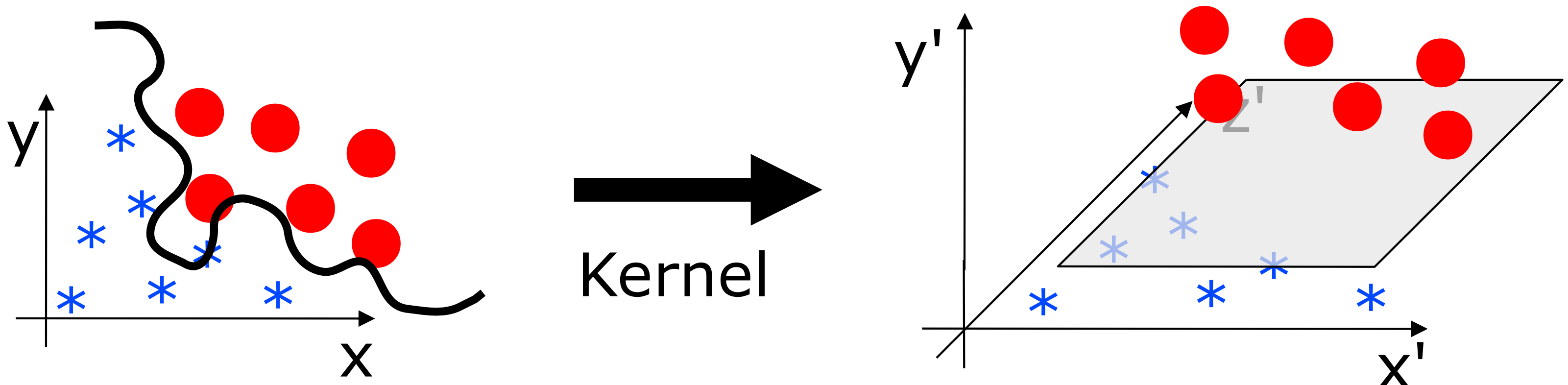
Success Story of LSTMs

- LSTMs have been used to win many competitions in speech and handwriting recognition.
- Major technology companies (Google, Apple, and Microsoft) are using LSTMs
  - Google used LSTM for speech recognition on the smartphone, for Google Translate.
  - Apple uses LSTM for the ”Quicktype” function on the iPhone and for Siri.
  - Amazon uses LSTM for Amazon Alexa.
  - In 2017, Facebook performed some 4.5 billion automatic translations every day using long short-term memory networks1.

RESERVOIR COMPUTING

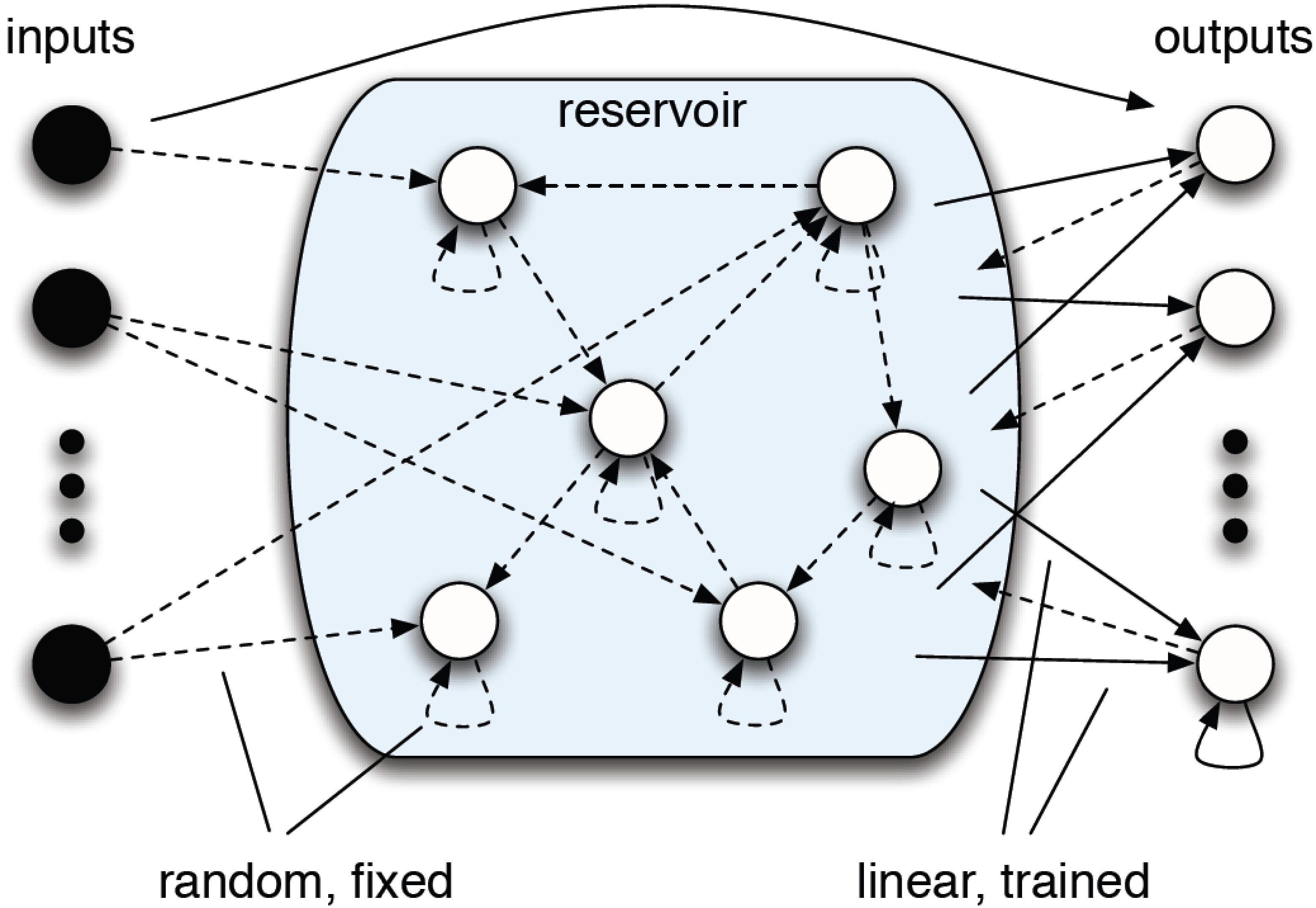
Reservoir Computing (RC): Idea

- Idea: Separate state space calculation from output calculation (as they serve different purposes)
  - Input (history) represented in high-dimensional state space (as for kernels used in SVMs)
  - Output spaces: Merger of states for desired output
- Uses recurrent structures without the training
  - Fixed (random) topology
  - Linear “readout” function is trained



Reservoir Computing: History

- Buonomano (1995), Laurenco (1994): early related work
- Boyd/Chua (95): Mathematical Foundation (without input feedback)
- Jaeger (2001): Echo State Networks (engineering)
- Maass (2002): Liquid State Machines (neuroscience)
- …
- And now: various physical reservoir computing approaches (morphological computing, cellular automata, etc.) (see Tanaka et al. 19))


inputs
outputs
reservoir
random, fixed
linear, trained

Reservoir Computing

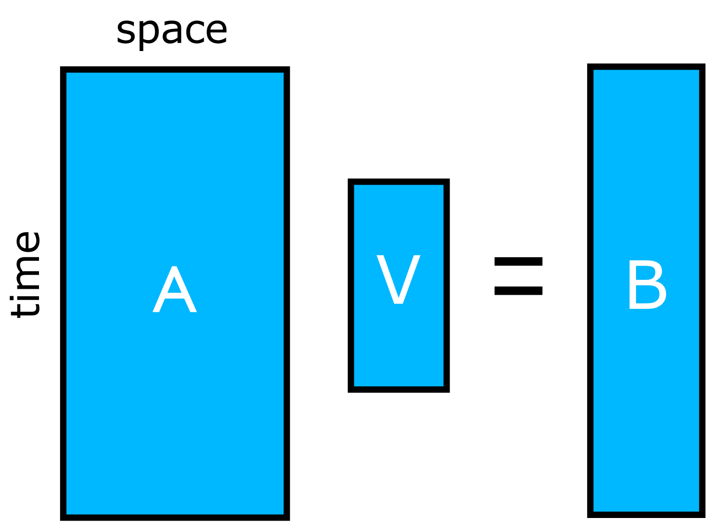
- (De-facto & required) Properties of reservoir:
  - Exact topology, connectivity, weights: not important
  - Has to have fading memory/echo state property: when not chaotic (as $k \to \infty$) effect of $h(t)$ and $x(t)$ on $h(t+k)$ vanishes
  - Can be ensured by choosing spectral radius of weight matrix (largest absolute eigenvalue) smaller than 1
  - Reservoir size can be large: no over-fitting
- Training with linear regression (or similar):
  - No local minima, no problems with recurrent structure, one shot learning
  - Can do regression, classification, prediction

Reservoir Computing

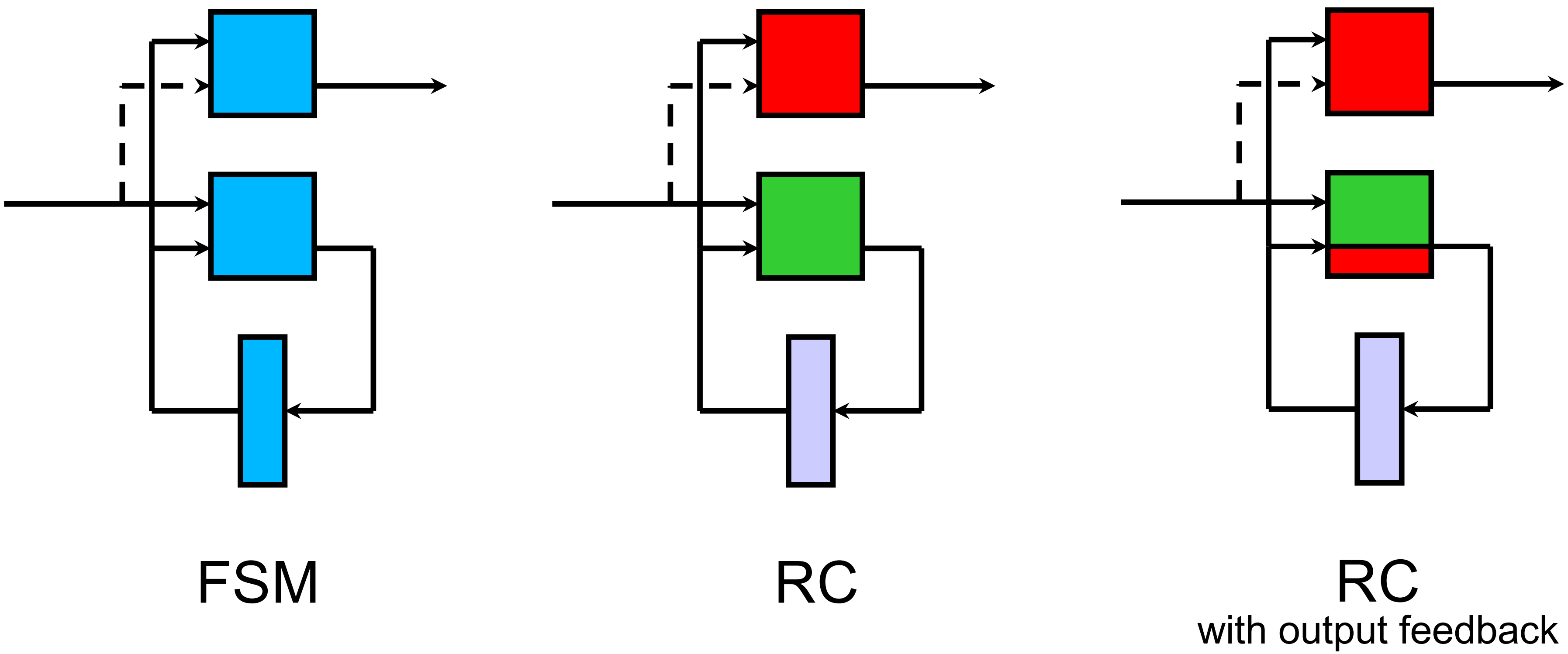
- RC does on-line computing: prediction at every time-step
- Theoretically:
  - Any time-invariant filter (F(x(t)) = F(x(t),t)) with fading memory can be learned
  - But: unable to implement generic FSMs
- Hence add output feedback, Maass (2006)
  - Also non-fading memory filters: generic FSMs
  - Ability to simulate any n-th order dynamical system
  - Turing universal

Usual setup and training

- Create random weight matrices
- Rescale reservoir weights so that max absolute eigenvalue close to one (edge of stability)
- Excite reservoir with input and record all states
- Train readouts by minimizing $(AV-B)^2$

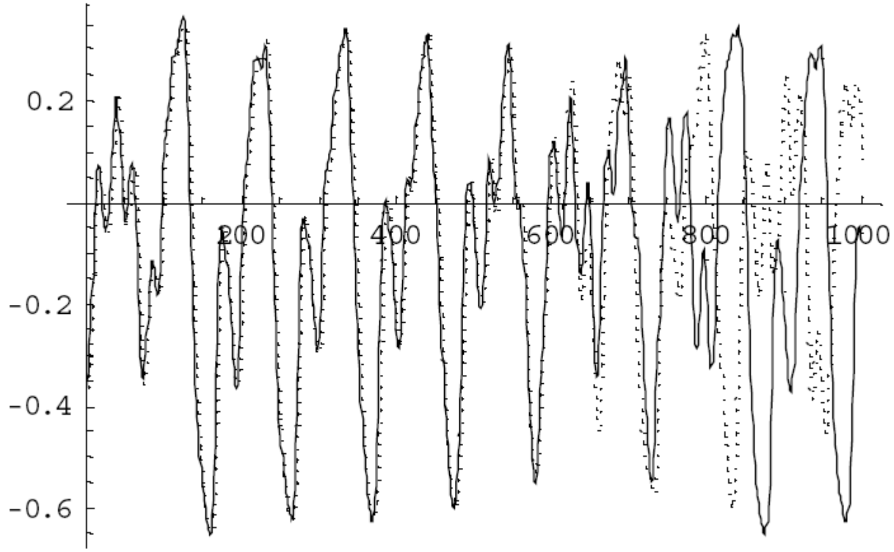


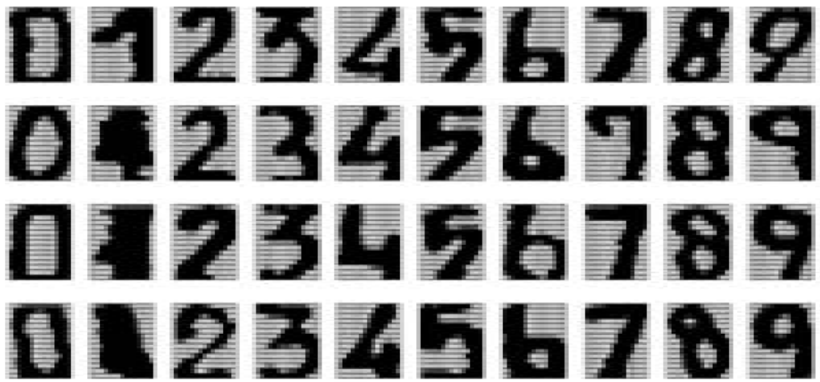
Link to FSMs



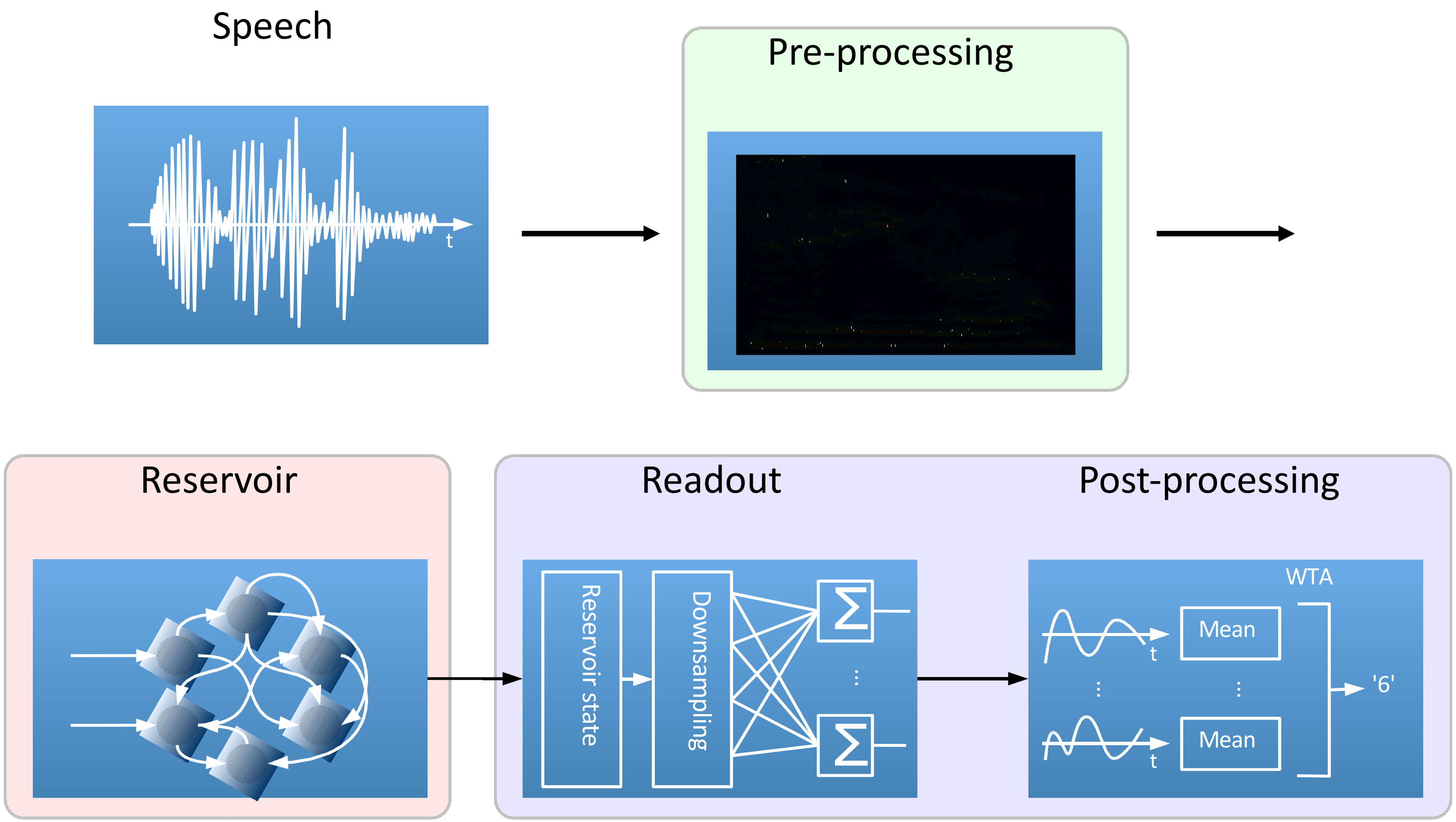
RC: Applications

- Chaotic time series prediction
- Speech recognition on small vocabulary: outperform HMM-based recognizer (Sphinx)
- Digits recognition
- Robot control
- System identification
- Noise removal/modelling
- …





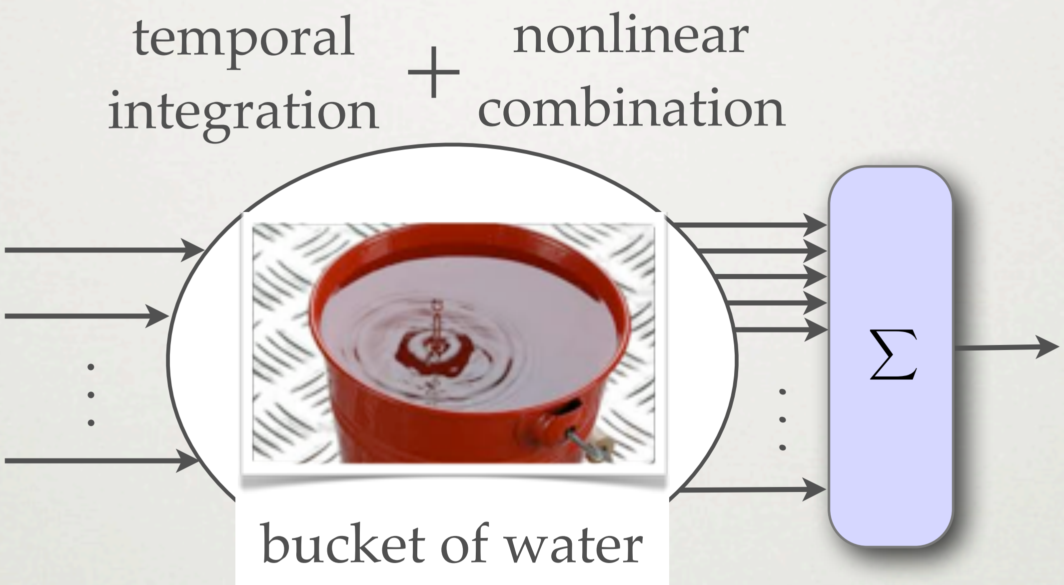
Larger example: speech



RC: novel computing paradigm

- RC presents a novel way of looking at computation
- "Random" dynamic systems can be used by only training a linear readout layer
- RC already used to show general computing capabilities of:
  - Microcolumn structure in the cortex
  - Gene regulatory network
  - The visual cortex of a real cat
- Implementations:
  - "Bucket of water", aVLSI, digital hardware
  - Photonics

Different Flavors of RC



- Water is mechanically perturbed (with motors)
- Complex response of the surface
- Readout is digitized picture frame + processing (vision)

Fernando and Sojakka, 2003

Uhhh, a lecture with a hopefully useful

APPENDIX

Color Convention in this course

- Formulae, when occurring inline
- Newly introduced terminology and definitions
- Important results (observations, theorems) as well as emphasizing some aspects
- Examples are given with standard orange with possibly light orange frame
- Comments and notes
- Algorithms

Today's lecture is based on the following

- Jonathon Hare: Lectures 12, 13 of course „COMP6248 Differentiable Programming (and some Deep Learning)"
  http://comp6248.ecs.soton.ac.uk/
- Michael Green & Shaked Perek: Recurrent networks And Long Short Term Memory link
- Karpathy: The unreasonable effectiveness of recurrent Neural Networks
  http://karpathy.github.io/2015/05/21/rnn-effectiveness/
- Benjamin Schrauven et al: An overview of reservoir computing, ESANN 2007 (paper and slides, link)
- Helmut Hauser, 2013: Introduction to Reservoir Computing
  https://www.ifi.uzh.ch/dam/jcr:00000000-2826-155d-0000-0000225e9316/Formale_Methoden_UZH_Nov_2013.pdf
- Deep Dive into deep learning, chapter 8
  https://d2l.ai/chapter_recurrent-neural-networks/bptt.html

References

- D. Buonomano and M. Merzenich. Temporal information transformed into a spatial code by a neural network with realistic properties. Science, 267(5200):1028–1030, 1995.
- S. Boyd and L. Chua. Fading memory and the problem of approximating nonlinear operators with volterra series. IEEE Transactions on Circuits and Systems, 32(11):1150–1161, 1985.
- G. Tanaka, T. Yamane, J. B. Heroux, R. Nakane, N. Kanazawa, S. Takeda, H. Numata, D. Nakano, and A. Hirose. Recent advances in physical reservoir computing: A review. Neural Networks, 115:100 –123, 2019.
- W. Maass, P. Joshi, and E. Sontag. Computational aspects of feedback in neural circuits. PLoS computational biology, 3(1):1–20, 2007.
- H. Jaeger. The"echo state"approach to analysing and training recurrent neural networks - gmd report. Technical Report 148, German National Research Center for Information Technology, Bonn, 2001.
- W. Maass, T. Natschläger, and H. Markram. Real-time computing without stable states: A new framework for neural computation based on perturbations. Neural Computation, 14(11):2531–2560, 2002.
- C. Fernando and S. Sojakka. Pattern recognition in a bucket. In W. Banzhaf, J. Ziegler, T. Christaller, P. Dittrich, and J. T. Kim, editors, Advances in Artificial Life, pages 588–597, Berlin, Heidelberg, 2003. Springer Berlin Heidelberg.