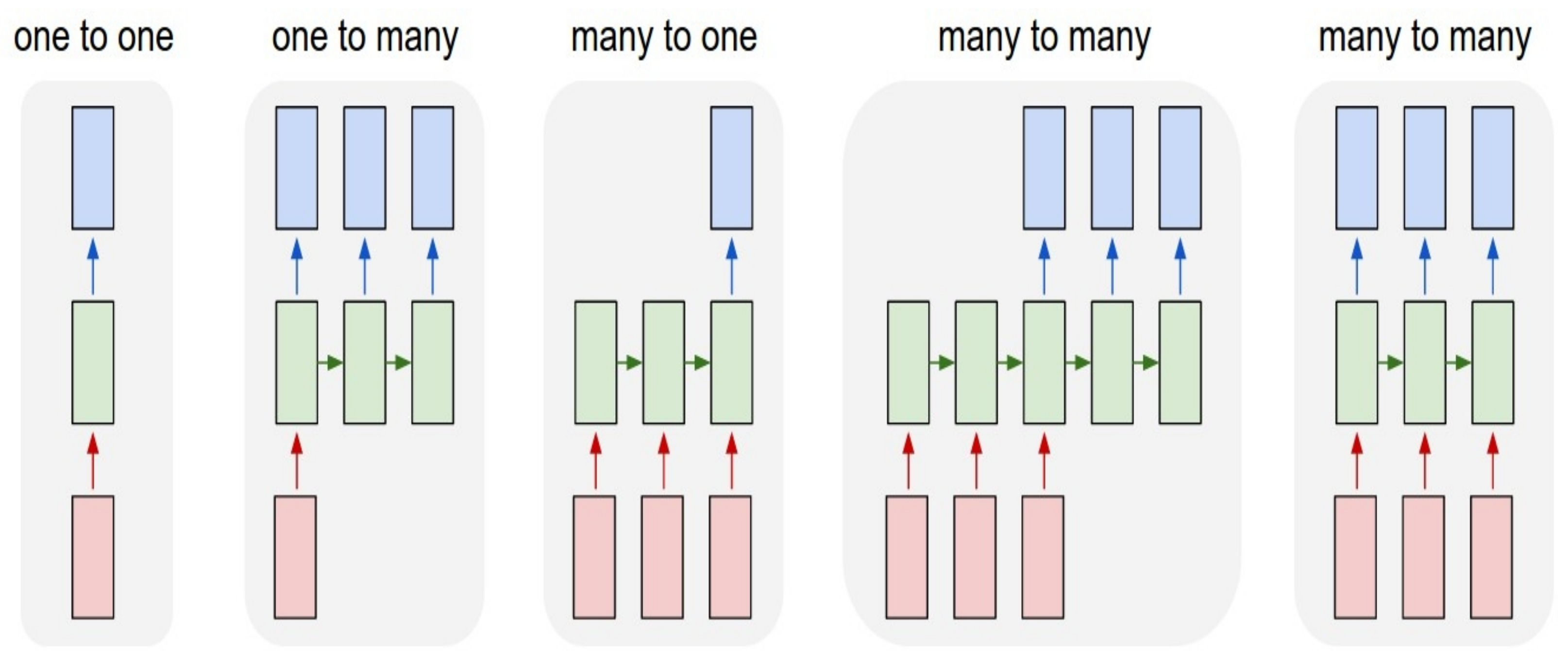
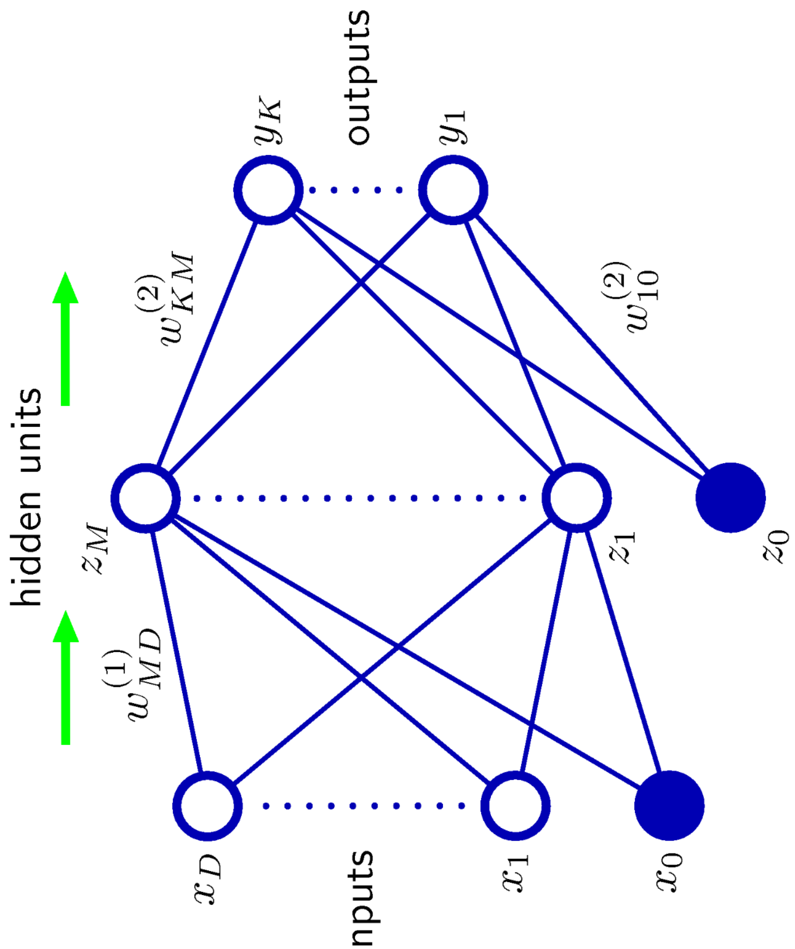
Introduction to
Recurrent Neural Networks

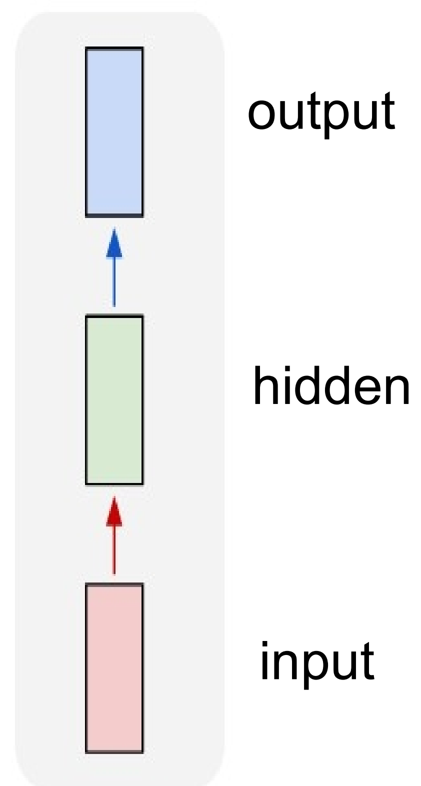
Jakob Verbeek



Modeling sequential data with Recurrent Neural Networks

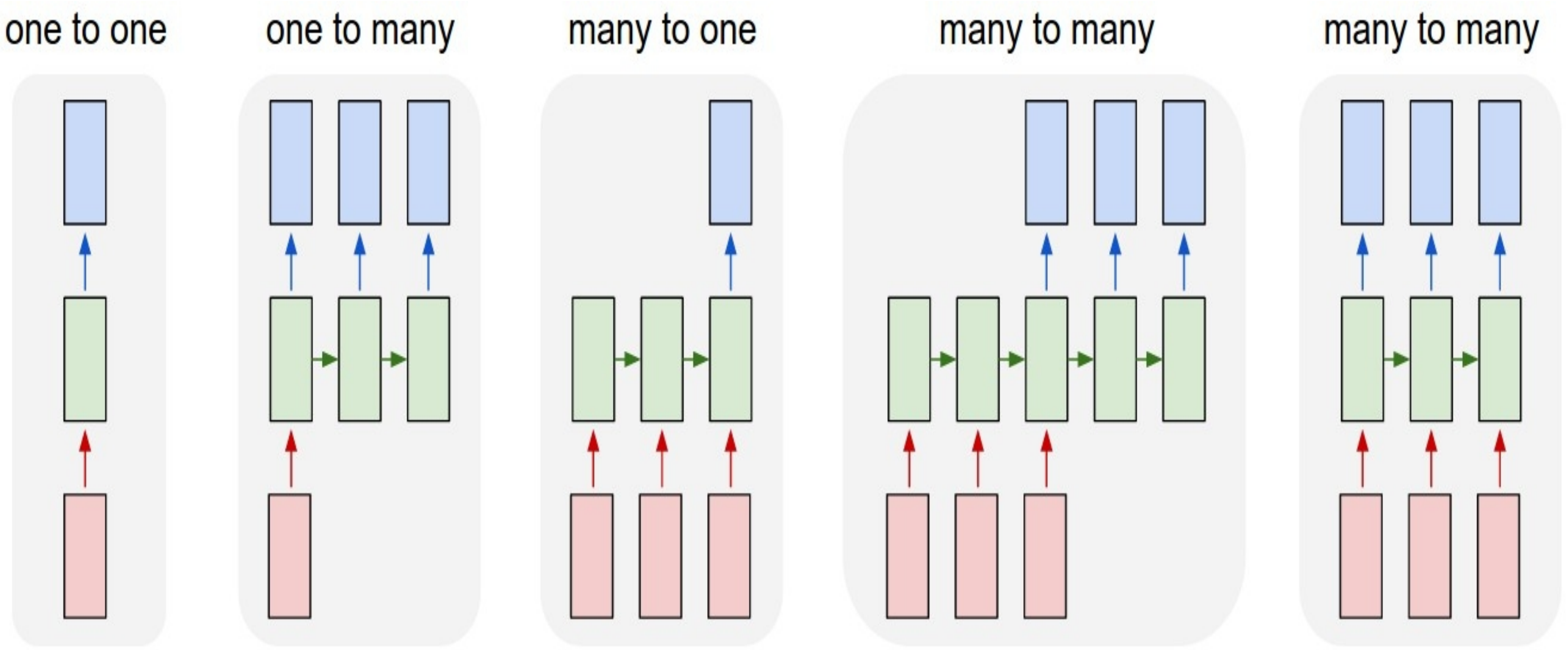
- Compact schematic drawing of standard multi-layer perceptron (MLP)





Modeling sequential data

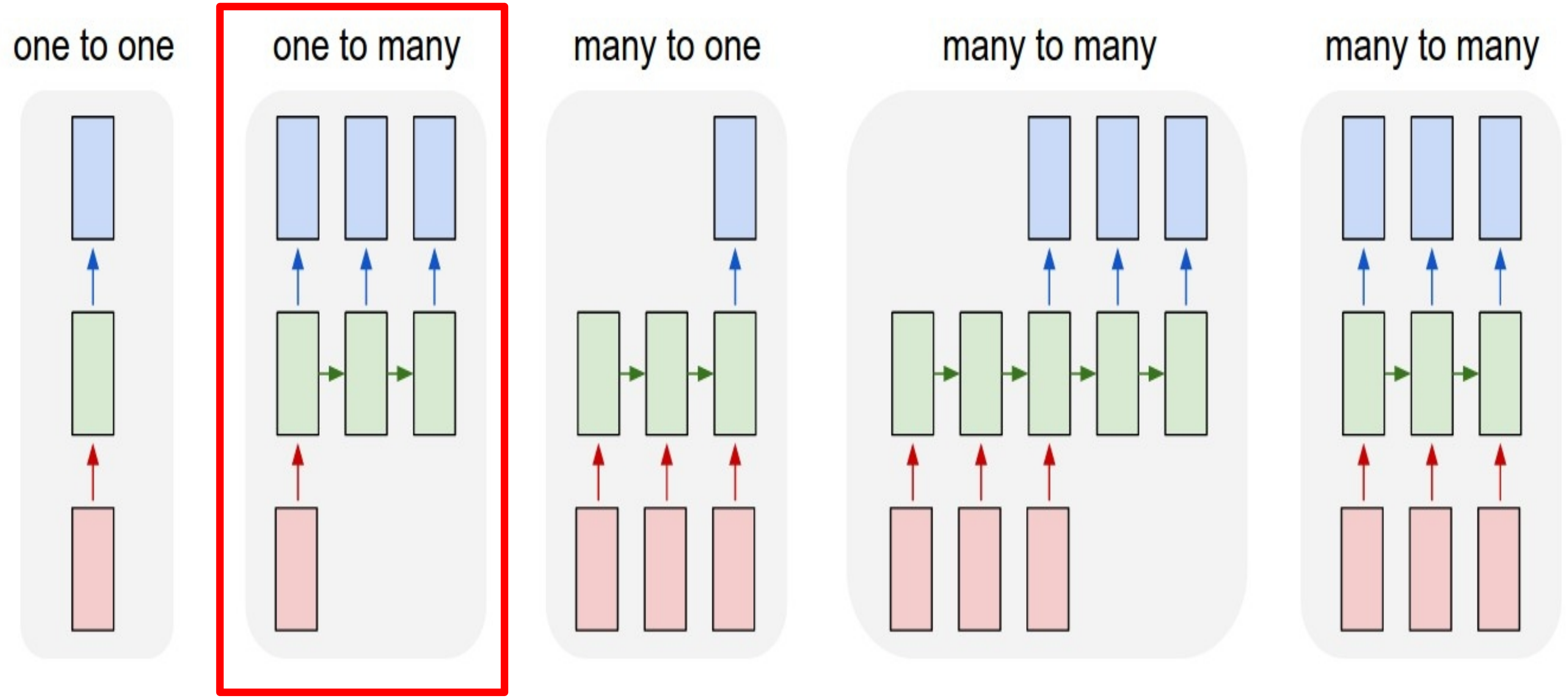
- So far we considered "one-to-one" prediction tasks
  - Classification: one image to one class label, which digit is displayed 0...9
  - Regression: one image to one scalar, how old is this person?
- Many prediction problems have a sequential nature to them
  - Either in input, in output, or both
  - Both may vary in length from one example to another



Modeling sequential data

- One-to-many prediction
- Image captioning
  - Input: an image
  - Output: natural language description, variable length sequence of words

a brown dog is running through the grass



Modeling sequential data

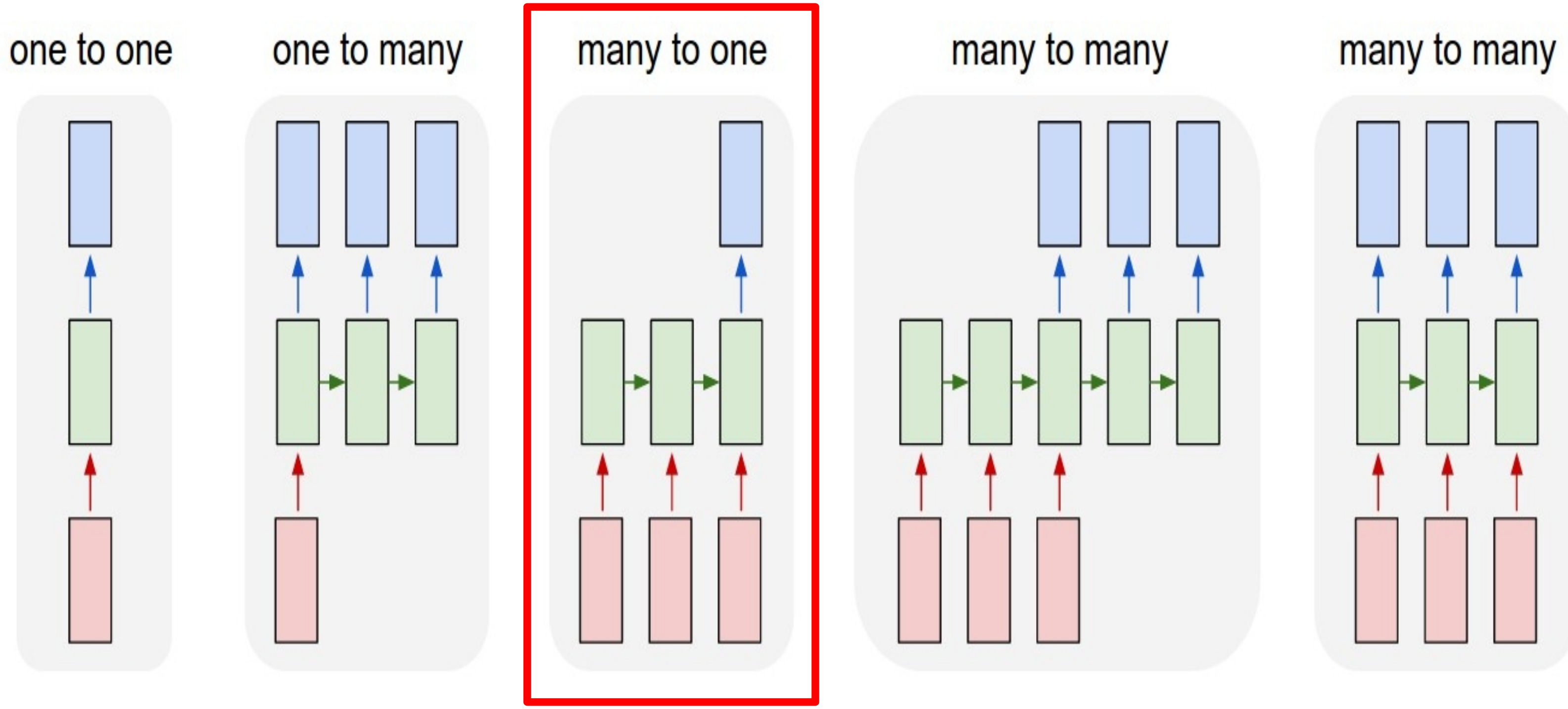
- Text classification
  - Input: a sentence
  - Output: user rating

I liked it...

Author: JustMeOnline from Portugal

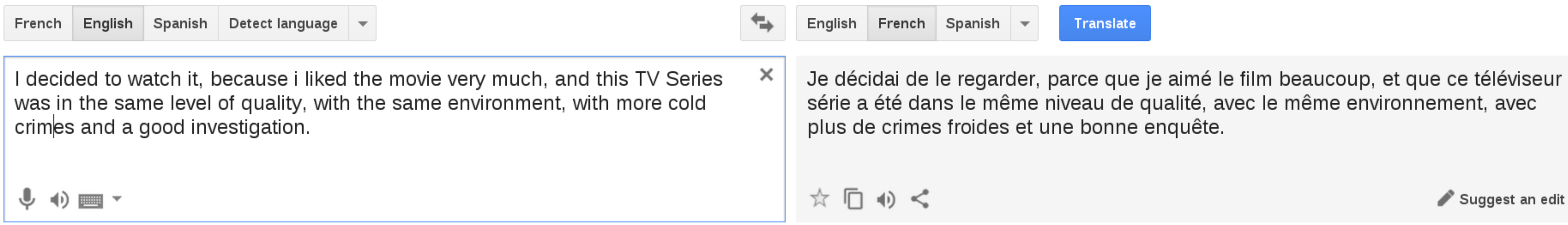
14 November 2014

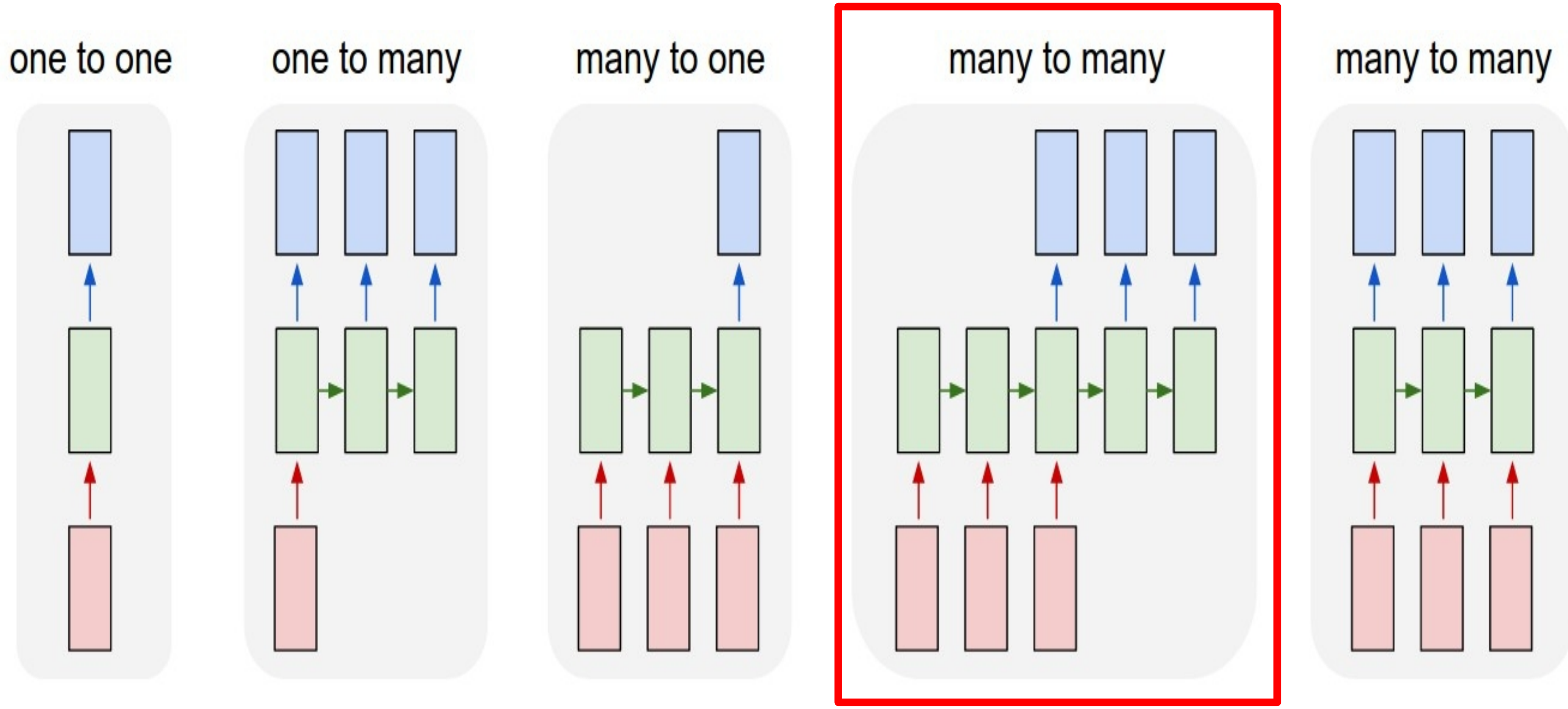
I decided to watch it, because i liked the movie very much, and this TV Series was in the same level of quality, with the same environment, with more cold crimes and a good investigation...



Modeling sequential data

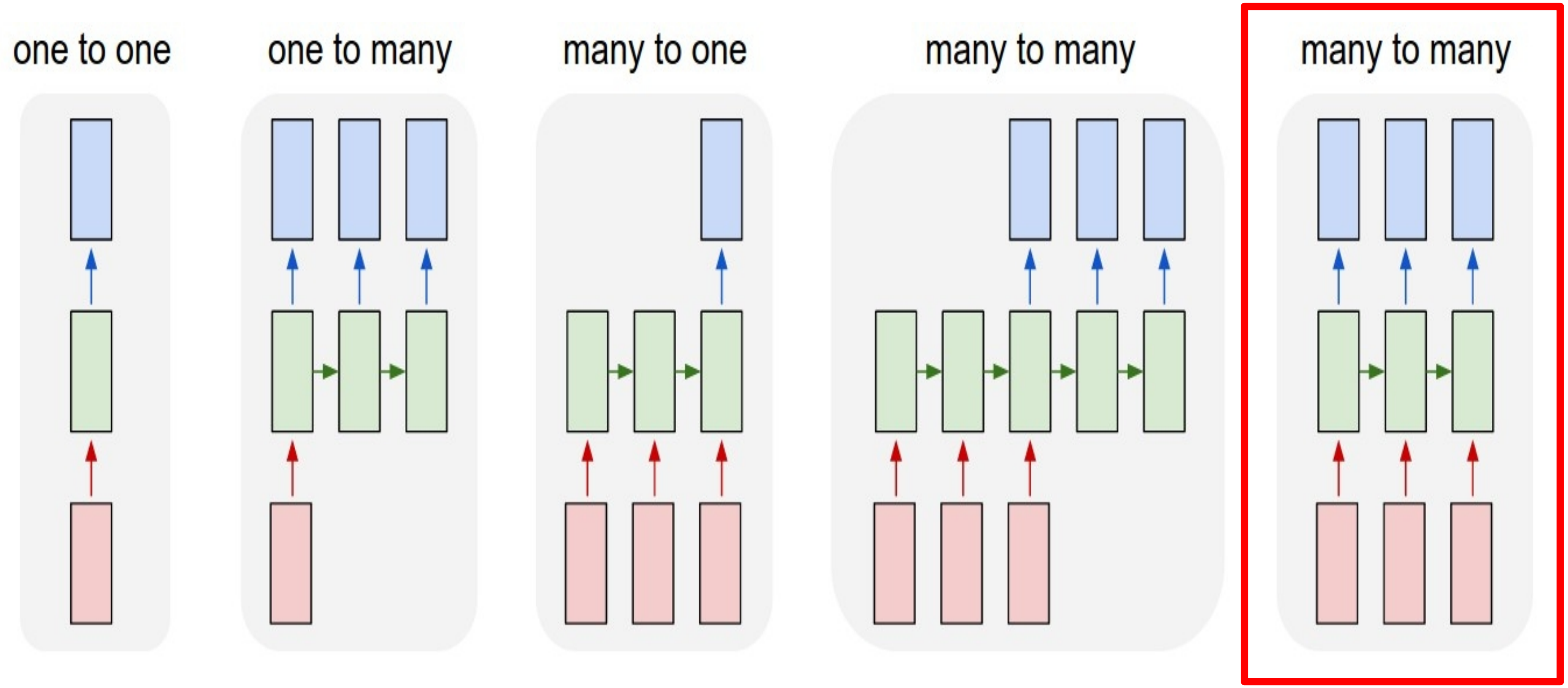
- Machine translation of text from one language to another
  - Sequences of different length on input and output





Modeling sequential data

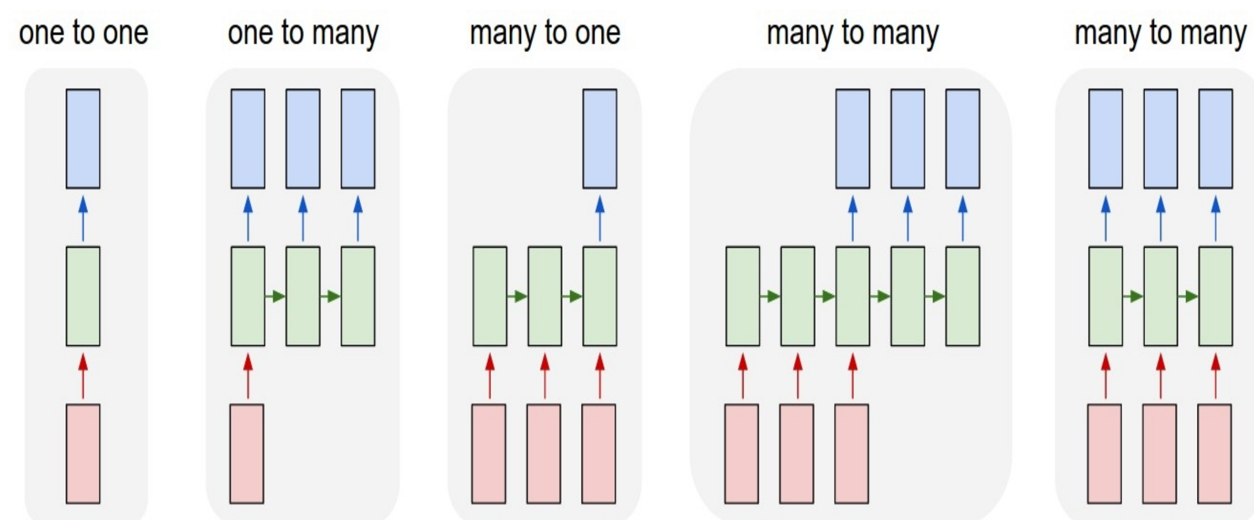
- Part of speech tagging
  - For each word in sentence predict PoS label (verb, noun, adjective, etc.)
- Temporal segmentation of video
  - Predict action label for every video frame
- Temporal segmentation of audio
  - Predict phoneme labels over time



Modeling sequential data

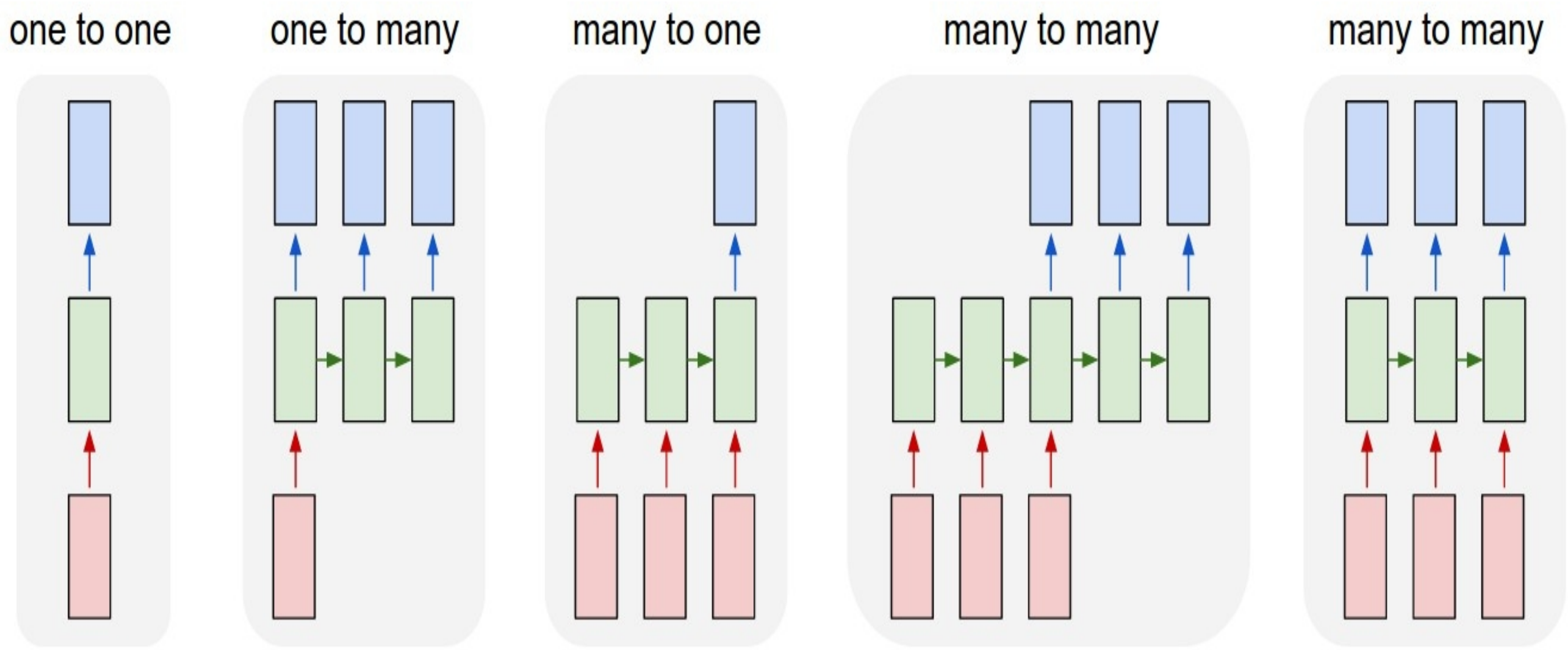
- Possible to use a k-order autoregressive model over output sequences
  - Limits memory to only k time steps in the past

- Not applicable when input sequence is not aligned with output sequence
  - Many-to-one tasks, unaligned many-to-many



Recurrent neural networks

- Recurrent computation of hidden units from one time step to the next
  - Hidden state accumulates information on entire sequence, since the field of view spans entire sequence processed so far
  - Time-invariant function makes it applicable to arbitrarily long sequences
- Similar ideas used in
  - Hidden Markov models for arbitrarily long sequences
  - Parameter sharing across space in convolutional neural networks
    - But has limited field of view: parallel instead of sequential processing

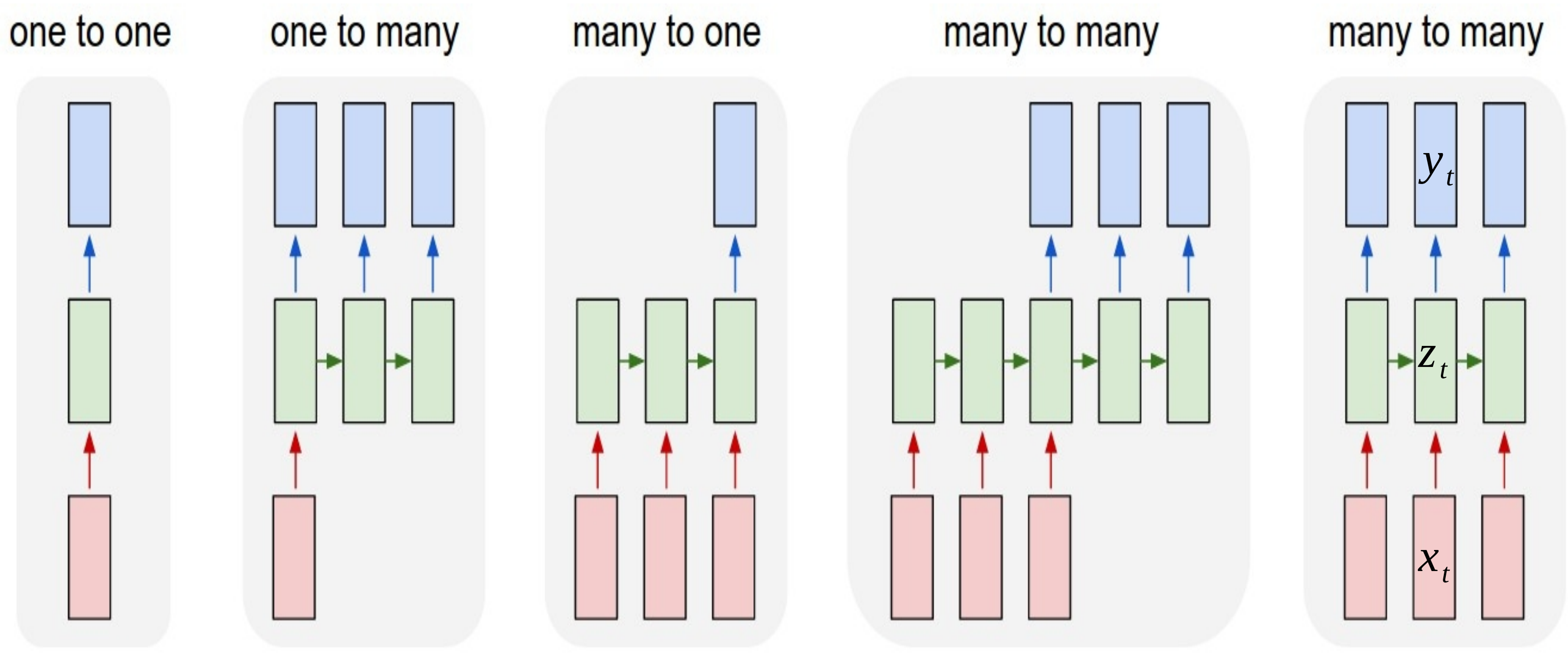


Recurrent neural networks

- Basic example for many-to-many prediction
  - Hidden state linear function of current input and previous hidden state, followed by point-wise non-linearity
  - Output is linear function of current hidden state, followed by point-wise non-linearity

$$z_t = \phi(A x_t + B z_{t-1})$$

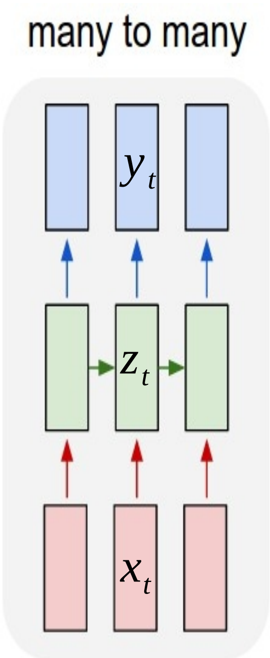
$$y_t = \psi(C z_t)$$



Recurrent neural network diagrams

- Two graphical representations are used

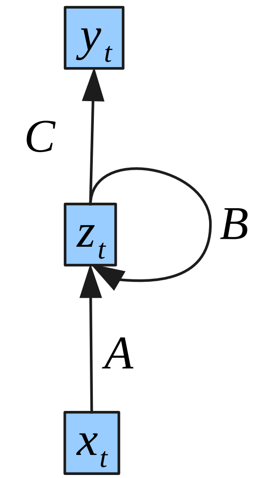
"Unfolded" flow diagram



$$z_t = \phi\left(A x_t + B z_{t-1}\right)$$

$$y_t = \psi\left(C z_t\right)$$

Recurrent flow diagram

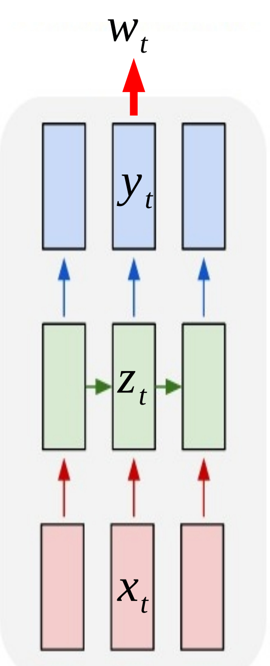


- Unfolded representation shows that we still have an acyclic directed graph
  - Size of the graph (horizontally) is variable, given by sequence length
  - Weights are shared across horizontal replications
- Gradient computation via back-propagation as before
  - Referred to as "back-propagation through time" (Pearlmutter, 1989)

Recurrent neural network diagrams

- Deterministic feed-forward network from inputs to outputs
- Predictive model over output sequence is obtained by defining a distribution over outputs given y
  - For example: probability of a word given via softmax of word score
- Training loss: sum of losses over output variables
  - Independent prediction of elements in output given input sequence

$$L = -\sum_{t=1}^{T} \ln p(w_t | x_{1:t})$$



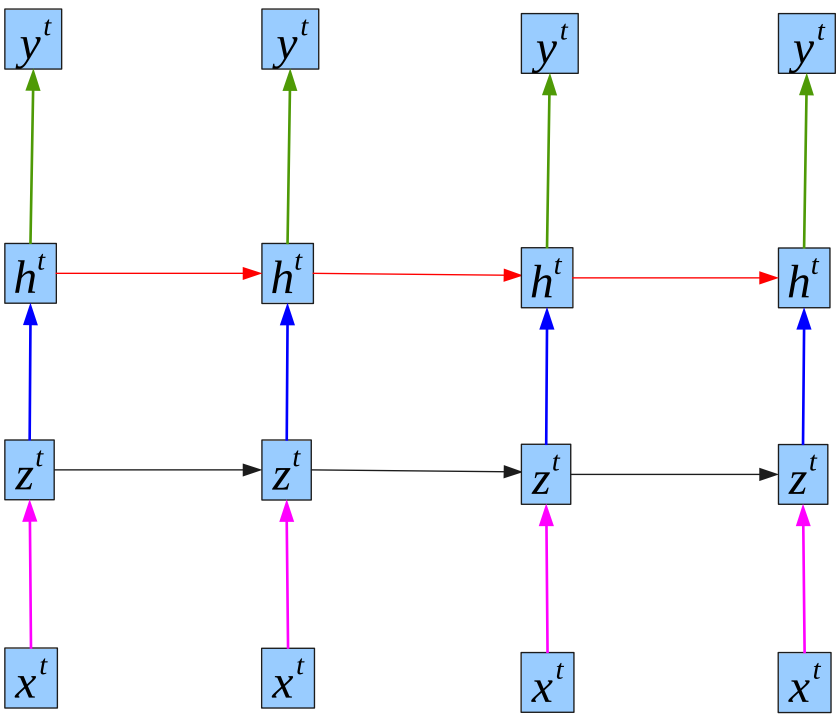
$$z_t = \phi(A x_t + B z_{t-1})$$

$$y_t = \psi(C z_t)$$

$$p(w_t = k | x_{1:t}) = \frac{\exp y_{tk}}{\sum_{v=1}^{V} \exp y_{tv}}$$

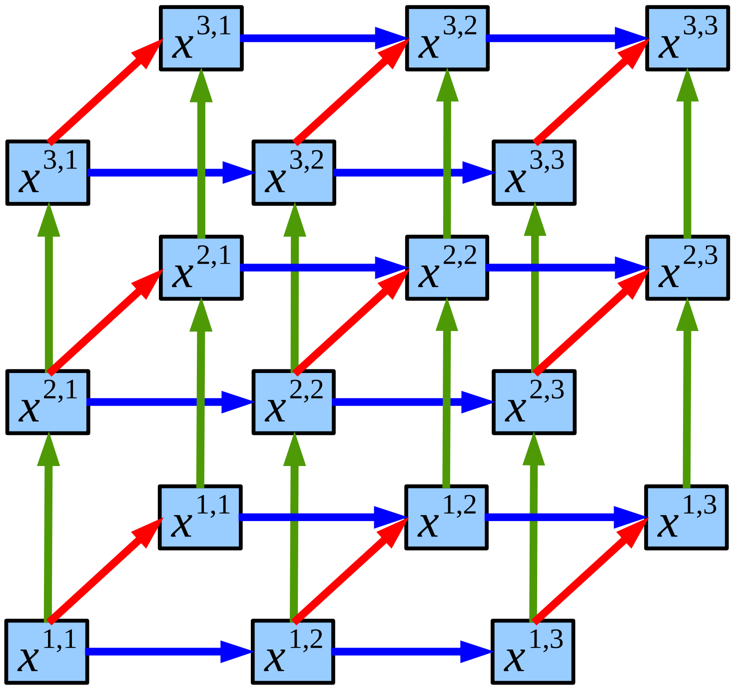
More topologies: “deep” recurrent networks

- Instead of a recurrence across a single hidden layer, consider a recurrence across a multi-layer architecture



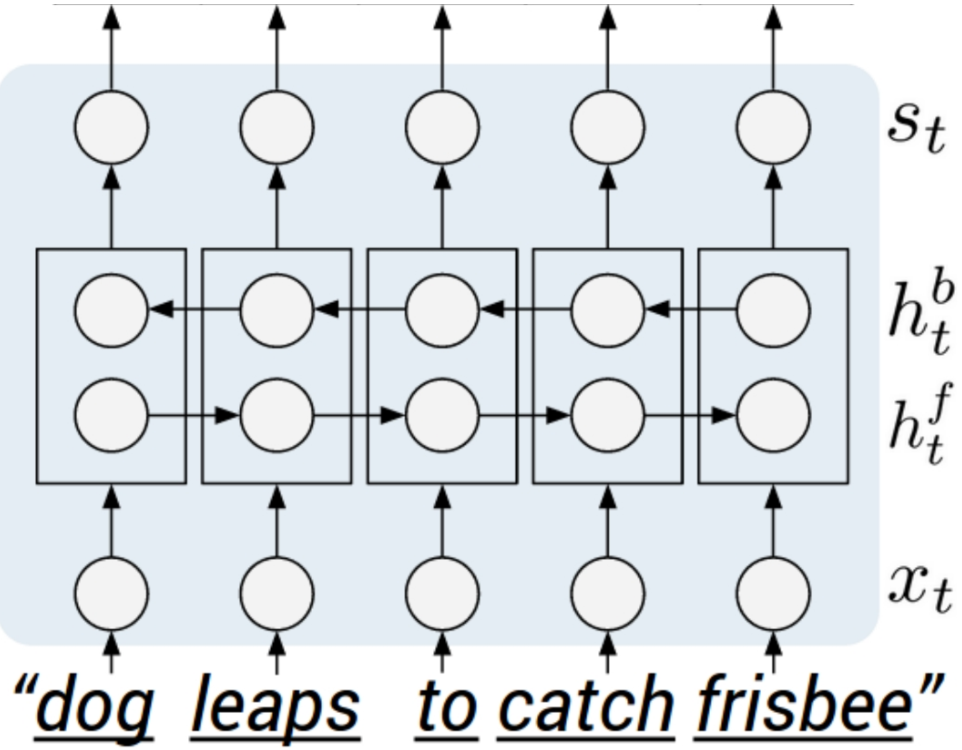
More topologies: multi-dimensional recurrent networks

- Instead of a recurrence across a single (time) axis, consider a recurrence across a multi-dimensional grid
- For example: axis aligned directed edges
  - Each node receives input from predecessors, one for each dimension



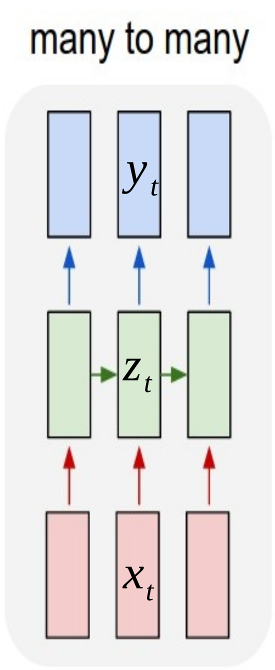
More topologies: bidirectional recurrent neural networks

- Standard RNN only uses left-context for many-to-many prediction
- Use two separate recurrences, one in each direction
  - Aggregate output from both directions for prediction at each time step
- Only possible on a given input sequence of arbitrary length
  - Not on output sequence, since it needs to be predicted/generated



More topologies: output feedback loops

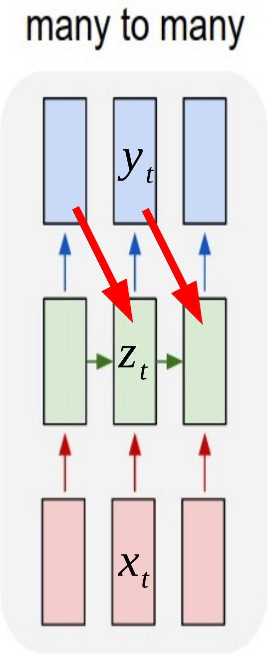
- So far the element in the output sequence at time t was independently drawn given the state at time t
  - State at time t depends on the entire input sequence up to time t
  - No dependence on the output sequence produced so far
- Problematic when there are strong regularities in output, eg character or words sequences in natural language



$$p(w_{1:T}|x_{1:T}) = \prod_{t=1}^{T} p(w_t|x_{1:t})$$

More topologies: output feedback loops

- To introduce dependence on output sequence, we add a **feedback loop** from the output to the hidden state



$$p(y_{1:T}|x_{1:T}) = \prod_{t=1}^{T} p(y_t|x_{1:t}, y_{1:t-1})$$

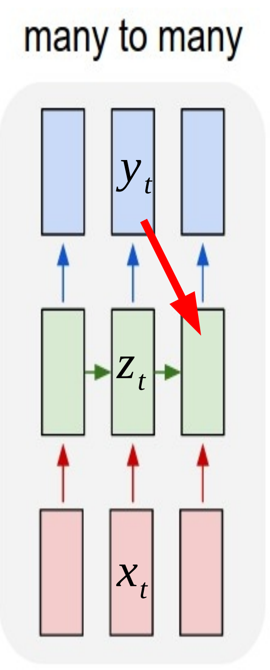
- Without output-feedback, the state evolution is a deterministic non-linear dynamical system
- With output feedback, the state evolution becomes a **stochastic non-linear dynamical system**
  - Caused by the stochastic output, which flows back into the state update

How do we generate data from an RNN ?

- RNN gives a distribution over output sequences

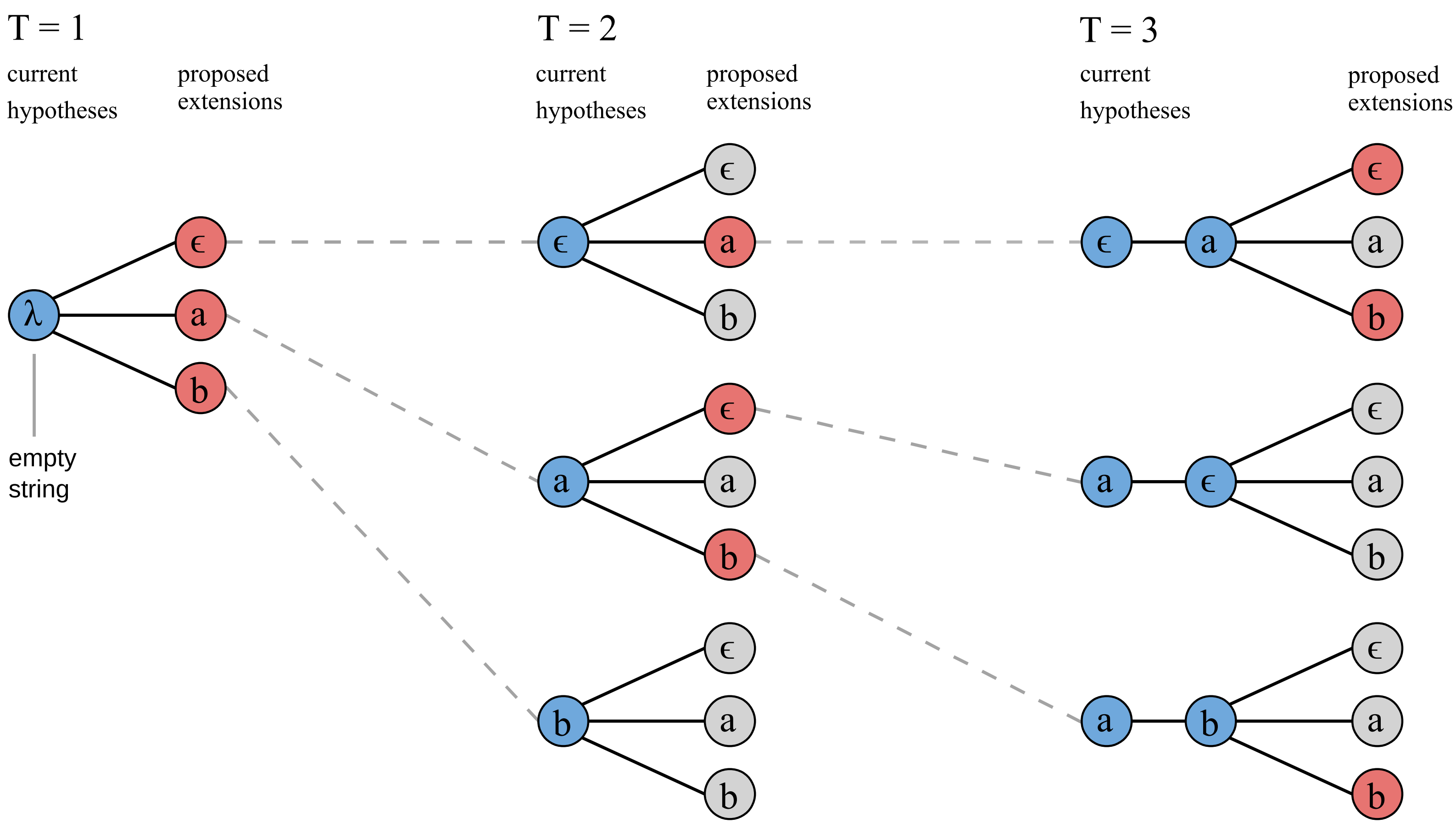
- Sampling: sequentially sample one element at a time
  - Compute state from current input and previous state and output
  - Compute distribution on current output symbol
  - Sample output symbol

- Compute maximum likelihood sequence?
  - Not feasible with feedback since output symbol impacts state
- Marginal distribution on n-th symbol
  - Not feasible: marginalize over exponential nr. of sequences
- Marginal probability of a symbol appearing anywhere in seq.
  - Not feasible: average over all marginals



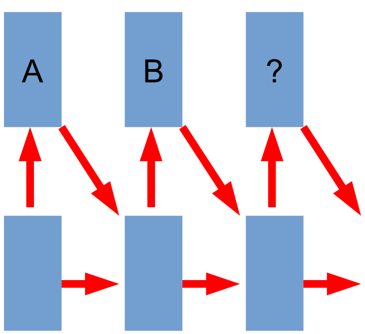
Approximate maximum likelihood sequences

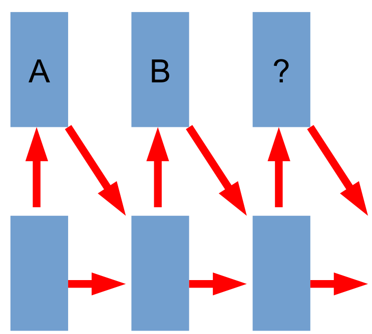
- Exhaustive maximum likelihood search exponential in sequence length
- Use Beam Search, computational cost linear in
  - Beam size K, vocabulary size V, (maximum) sequence length T



Ensembles of networks to improve prediction

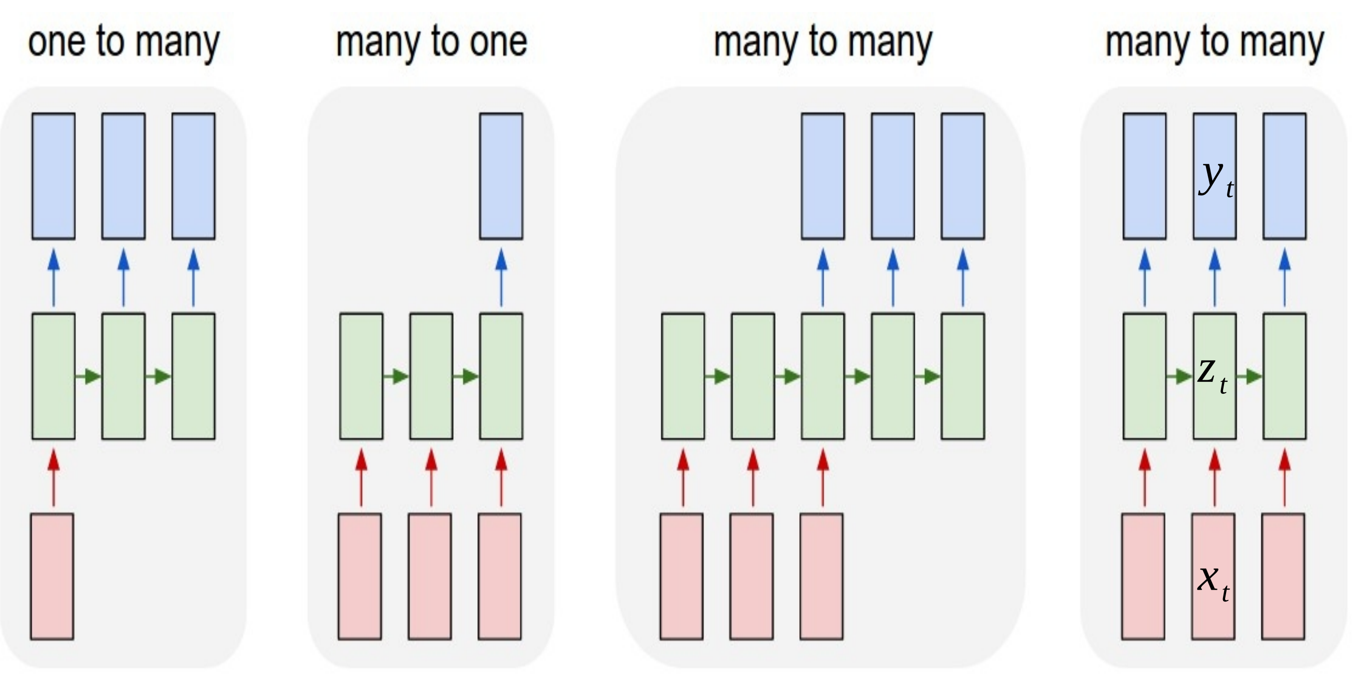
- Averaging predictions of several networks can improve results
  - Trained from different initialization and using different mini-batches
  - Possibly including networks with different architectures, but not per se
  - For CNNs see eg [Krizhevsky & Hinton, 2012] [Simomyan & Zisserman, 2014]
- For RNN sequence prediction
  - Train RNNs independently
  - "Run" RNNs in parallel for prediction, updating states with common seq.
  - Average distribution over next symbol
  - Sample or beam-search based on av. distribution





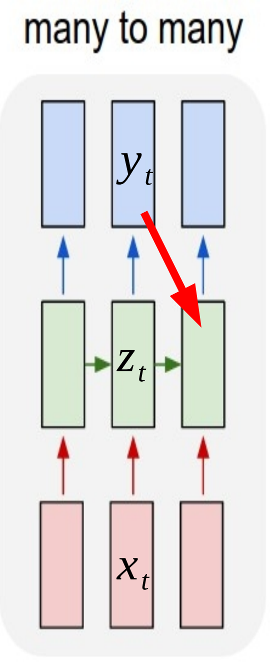
How to train an RNN without output feedback?

- Compute full state sequence given the input (deterministic given input)
- Compute loss at each time step w.r.t. ground truth output sequence
- Backpropagation ("through time") to compute gradients w.r.t. loss



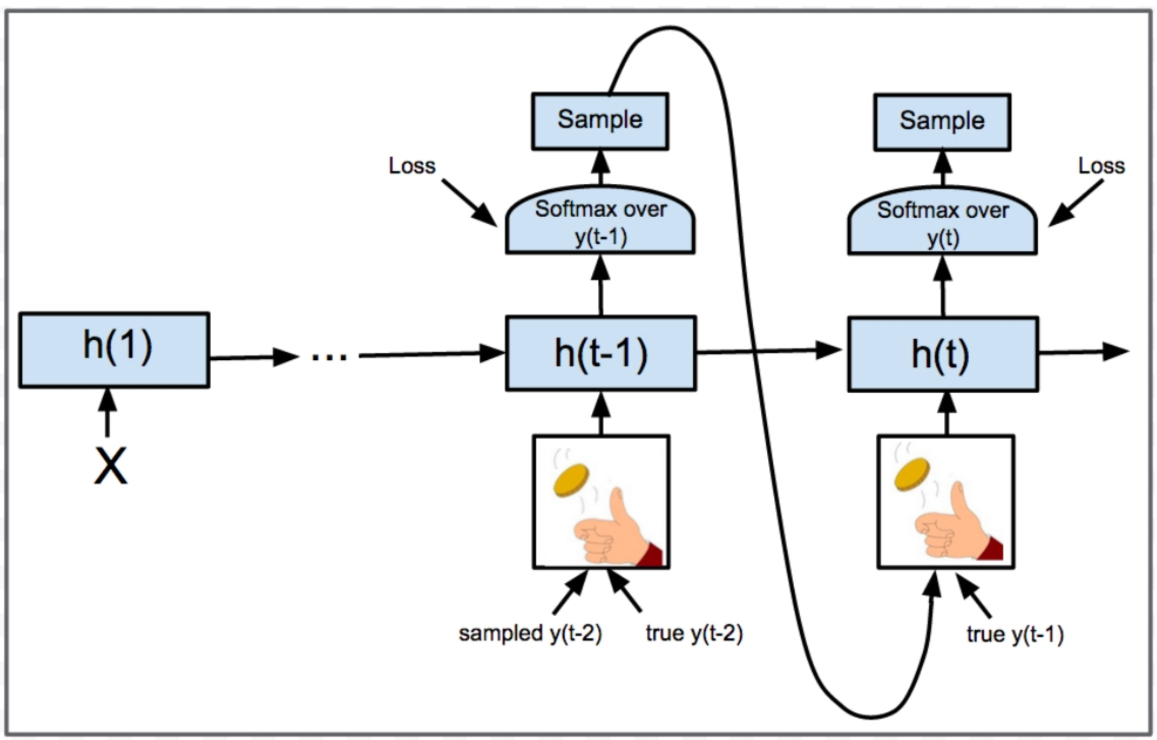
How to train an RNN with output feedback?

- Compute state sequence given input **and ground-truth output, deterministic due to known and fixed output**
- Loss at each time step wrt ground truth output seq, backprop through time
- Note discrepancy between train and test
  - Train: predict next symbol from **ground-truth sequence** so far
  - Test: predict next symbol from **generated sequence** so far
    - Might deviate from observed ground-truth sequences



Scheduled sampling for RNN training

- Compensate discrepancy between train and test procedure by training from generated sequence [Bengio et al. NIPS, 2015]
  - Learn to recover from partially incorrect sequences
- Directly training from sampled sequences does not work well in practice
  - At the start randomly initialized model generates random sequences
  - Instead, start by training from ground-truth sequence, and progressively increase probability to sample generated symbol in the sequence



Scheduled sampling for RNN training

- Evaluation image captioning
  - Image in, sentence out
  - Higher scores are better
- Scheduled sampling improves baseline, also in ensemble case
- Uniform Scheduled Sampling: sample uniform instead of using model
  - Already improves over baseline, but not as much as using model
- Always sampling gives very poor results, as expected

Approach vs Metric	BLEU-4	METEOR	CIDER
Baseline	28.8	24.2	89.5
Baseline with Dropout	28.1	23.9	87.0
Always Sampling	11.2	15.7	49.7
Scheduled Sampling	**30.6**	**24.3**	**92.1**
Uniform Scheduled Sampling	29.2	24.2	90.9
Baseline ensemble of 10	30.7	25.1	95.7
Scheduled Sampling ensemble of 5	**32.3**	**25.4**	**98.7**

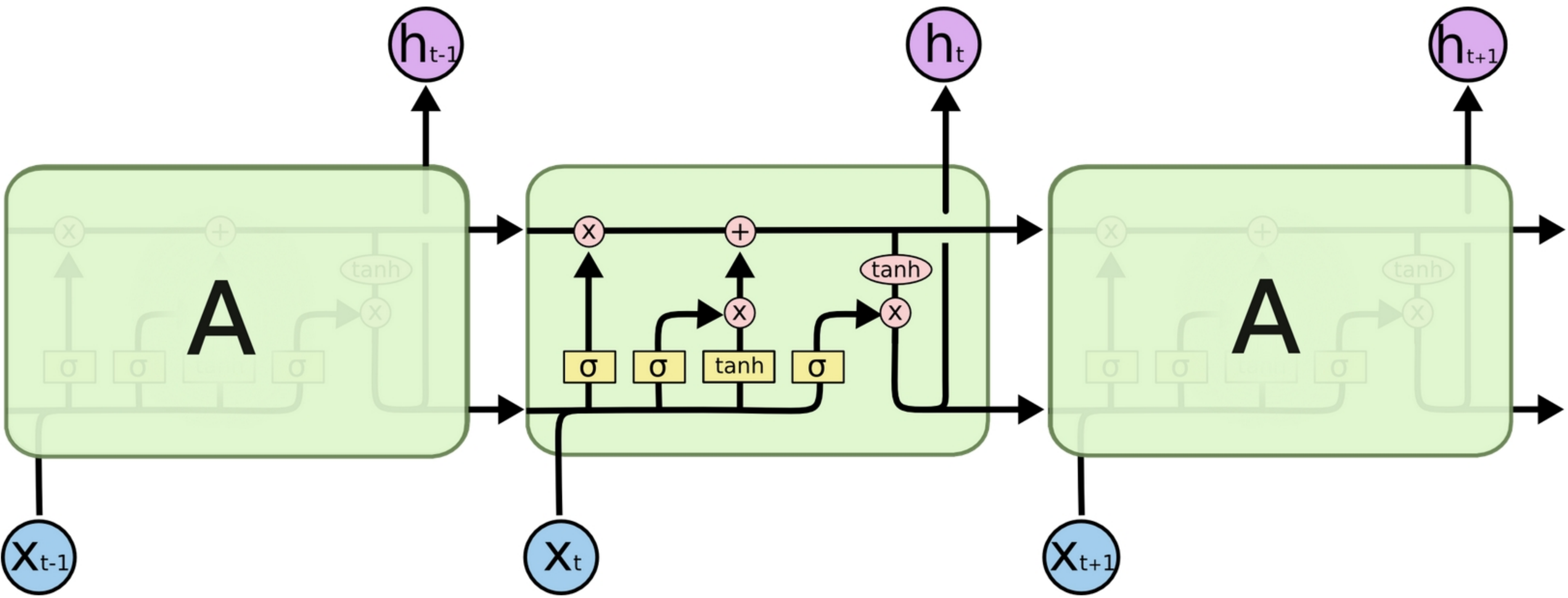
Limitations recurrent networks

- Recurrent net can be unrolled as deep network with shared parameters
  - As deep as the number of time steps of the RNN
  - Very deep for very long sequences
- Gradients of “deep” layers (far from input) computed via chainrule as product of Jacobians between layers (time-steps)
  - Product of Jacobians tend to either “explode” to inf. or “vanish” to zero
  - Similar effect observed in non-recurrent networks
- Approaches to address this issue
  - Non-recurrent case: add skip connections from earlier layers towards output: Residual networks, dense networks
  - Introduction of “gates” that shield a hidden unit from input and/or output for several layers, effectively shortening the depth for that unit

Long short-term memory (LSTM) cells

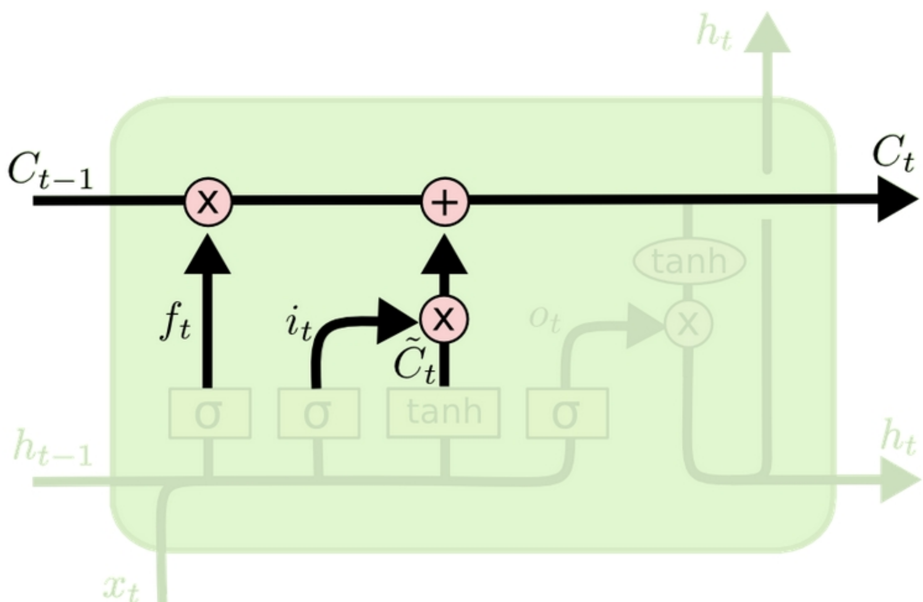
- LSTM consist of hidden state **h** and a “memory cell” **c**
- Gates are used to modulate the state updates

  [Hochreiter & Schmidhuber, Neural Computation, 1997]



Long short-term memory (LSTM) cells

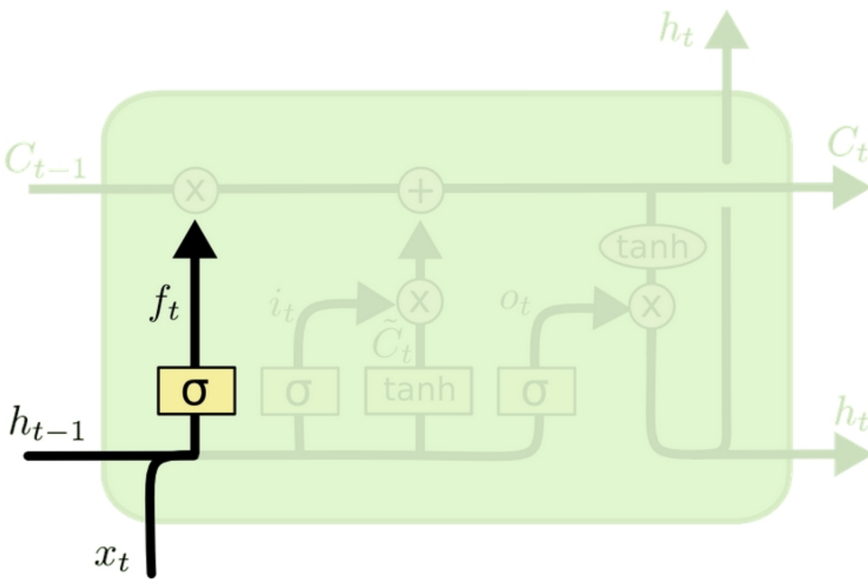
- Introduced by Hochreiter & Schmidhuber (Neural Computation, 1997)
- LSTM defines a dynamical system on hidden state h and a "memory cell" **c**
- Involves a number of additional processing elements
    - Cell update: can forget previous cell state, can ignore input



$$C_t = \boxed{f_t} * C_{t-1} + \boxed{i_t} * \tilde{C}_t$$

Long short-term memory (LSTM) cells

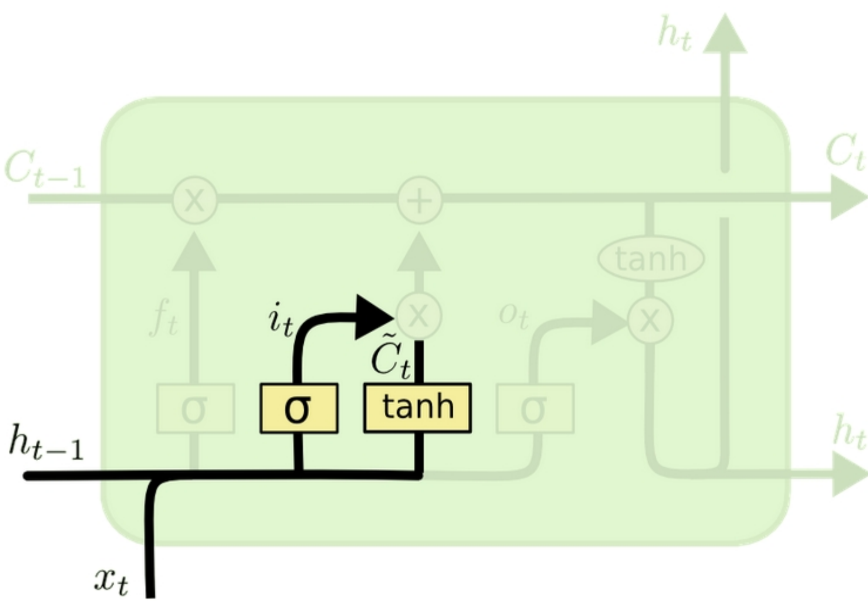
- Introduced by Hochreiter & Schmidhuber (Neural Computation, 1997)
- LSTM defines a dynamical system on hidden state **h** and a "memory cell" **c**
- Involves a number of additional processing elements
  - Forget gate **f:** "remember" or "forget" previous cell state **c**



$$f_t = \sigma\left(W_f \cdot [h_{t-1}, x_t] + b_f\right)$$

Long short-term memory (LSTM) cells

- Introduced by Hochreiter & Schmidhuber (Neural Computation, 1997)
- LSTM defines a dynamical system on hidden state h and a "memory cell" **c**
- Involves a number of additional processing elements
  - Input gate **i**: controls flow of input to cell state
  - Input modulator $\tilde{C}$, maps input and previous state to cell state update

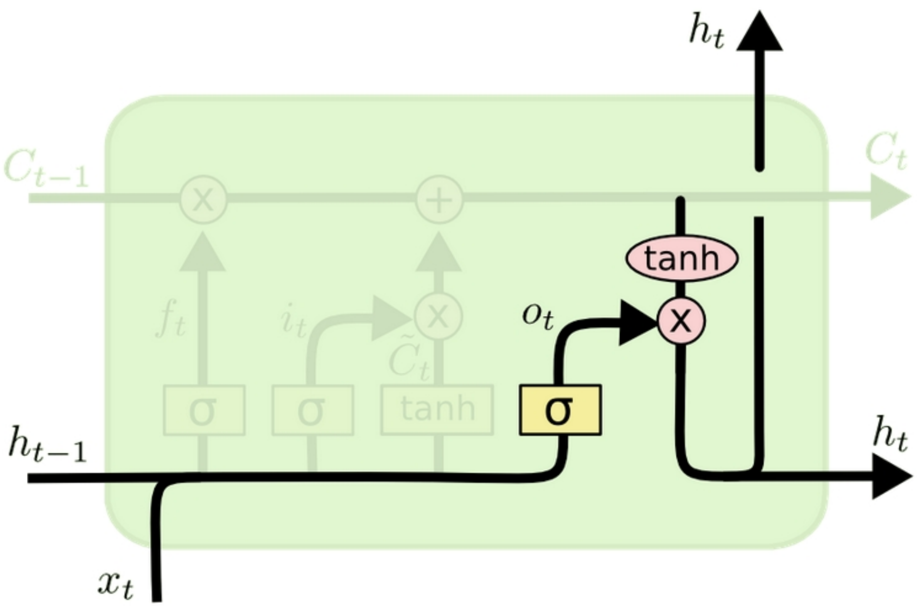


$$i_t = \sigma \left(W_i \cdot [h_{t-1}, x_t] \ + \ b_i \right)$$

$$\tilde{C}_t = \tanh(W_C \cdot [h_{t-1}, x_t] \ + \ b_C)$$

Long short-term memory (LSTM) cells

- Introduced by Hochreiter & Schmidhuber (Neural Computation, 1997)
- LSTM defines a dynamical system on hidden state h and a “memory cell” **c**
- Involves a number of additional processing elements
  - Output gate **o**, controls flow of cell state to output
  - Output vector also passed to next time step of LSTM unit

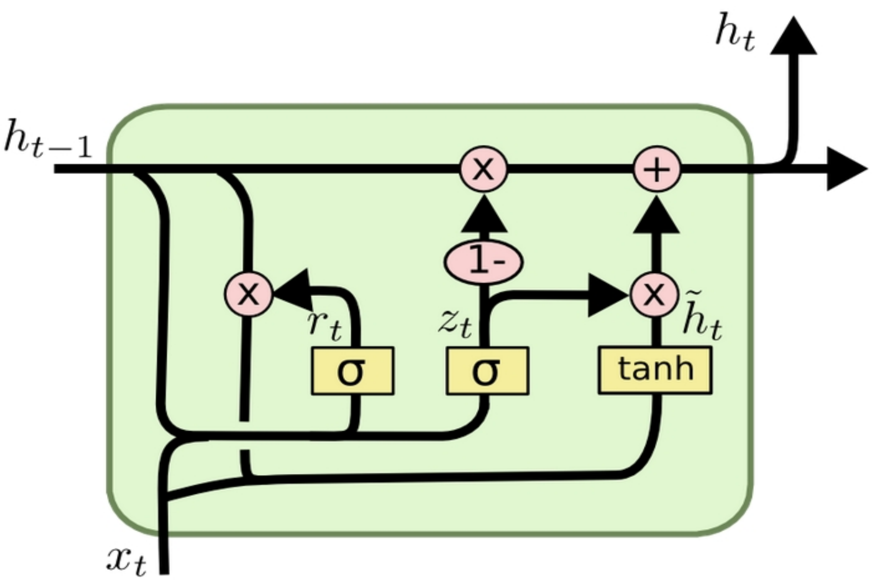


$$o_t = \sigma\left(W_o\ [h_{t-1}, x_t]\ +\ b_o\right)$$

$$h_t = o_t * \tanh\left(C_t\right)$$

Gated Recurrent Unit (GRU) cells

- GRU is simplified gated RNN as compared to LSTM
  [Cho et al., Empirical Methods in Natural Language Processing, 2014]
- Two gates, single state signal
  - Forget gate: **z**
  - Read gate: **r**



$$z_t = \sigma\left(W_z \cdot [h_{t-1}, x_t]\right)$$

$$r_t = \sigma\left(W_r \cdot [h_{t-1}, x_t]\right)$$

$$\tilde{h}_t = \tanh\left(W \cdot [r_t * h_{t-1}, x_t]\right)$$

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

Examples of character-level LSTM language model

- Training data: all Paul Graham essays, about 1 million characters
- Random sample from the trained model:

  "The surprised in investors weren't going to raise money. I'm not the company with the time there are all interesting quickly, don't have to get off the same programmers. There's a super-angel round fundraising, why do you can do. If you have a different physical investment are become in people who reduced in a startup with the way to argument the acquirer could see them just that you're also the founders will part of users' affords that and an alternation to the idea. [2] Don't work at first member to see the way kids will seem in advance of a bad successful startup. And if you have to act the big company too."

- Learns to spell words, as well as long range grammatical dependencies

[examples taken from Andrej Karpathy]

Examples of character-level LSTM language model

- Training data: all of Shakespeak (4.4 MB)
- Random sample from the trained model:

PANDARUS:
Alas, I think he shall be come approached and the day
When little srain would be attain'd into being never fed,
And who is but a chain and subjects of his death,
I should not sleep.

Second Senator:
They are away this miseries, produced upon my soul,
Breaking and strongly should be buried, when I perish
The earth and thoughts of many states.

DUKE VINCENTIO:
Well, your wit is in the care of side and that.

Second Lord:
They would be ruled after this chamber, and
my fair nues begun out of the fact, to be conveyed,
Whose noble souls I'll have the heart of the wars.

Clown:
Come, sir, I will make did behold your worship.

VIOLA:
I'll drink it.

- Specific style structure is also captured by the model

Examples of character-level LSTM language model

- Training data: linux source code (474 MB)
- Very long range dependencies on bracket structure

```
/*
 * Increment the size file of the new incorrect UI_FILTER group information
 * of the size generatively.
 */
static int indicate_policy(void)
{
  int error;
  if (fd == MARN_EPT) {
    /*
     * The kernel blank will coeld it to userspace.
     */
    if (ss->segment < mem_total)
      unblock_graph_and_set_blocked();
    else
      ret = 1;
    goto bail;
  }
  segaddr = in_SB(in.addr);
  selector = seg / 16;
  setup_works = true;
  for (i = 0; i < blocks; i++) {
    seq = buf[i++];
    bpf = bd->bd.next + i * search;
    if (fd) {
      current = blocked;
    }
  }
  rw->name = "Getjbbregs";
  bprm_self_clearl(&iv->version);
  regs->new = blocks[(BPF_STATS << info->historidac)] | PFMR_CLOBATHINC_SECONDS << 12;
  return segtable;
}
```

Case study: image captioning

- Given image generate descriptive english sentence

a brown dog is running through the grass

Image captioning with encoder-decoder system

- Encoder: CNN takes image and maps it into a vector
- For example, fully connected layer of VGG16 network
  - CNN pre-trained on ImageNet classification task (>1 million images)

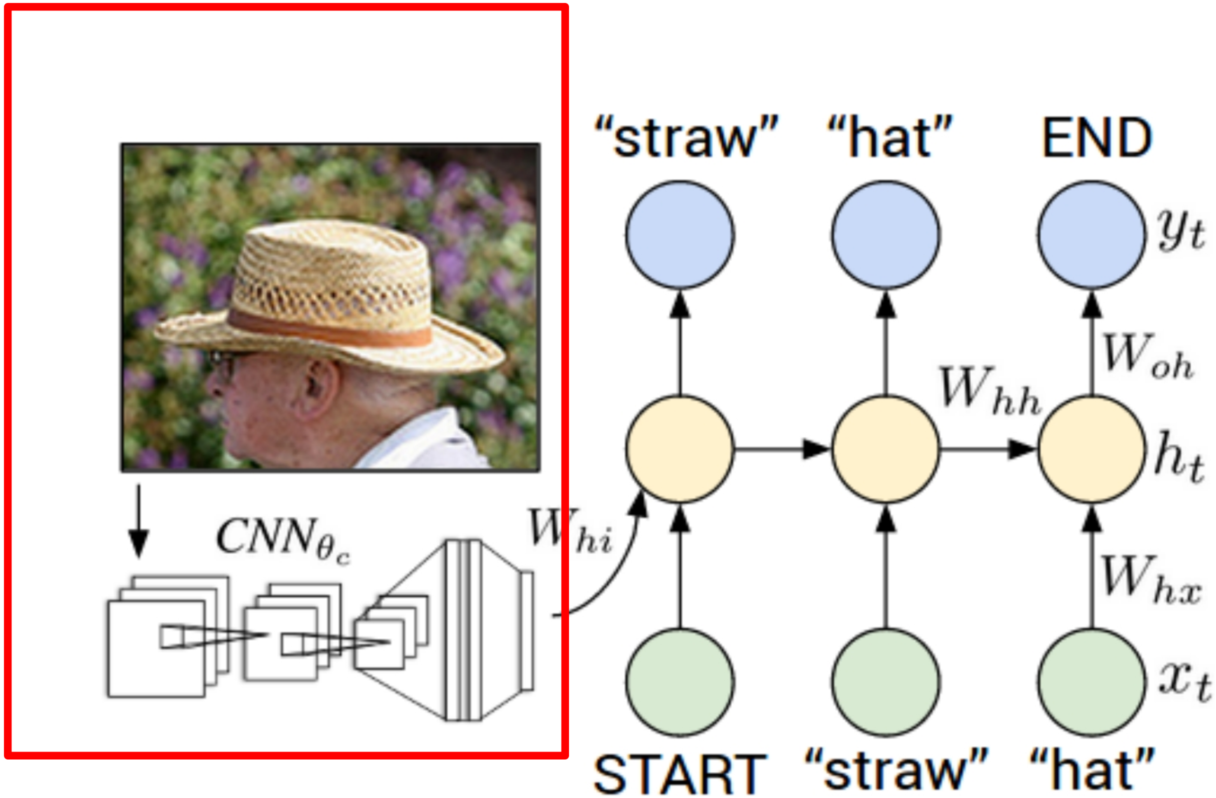


Image captioning with encoder-decoder system

- Decoder: RNN takes CNN image vector to initialize RNN state
- Typical configuration:
  - Single layer of 512 GRUs
  - Output feedback to ensure coherent sentence

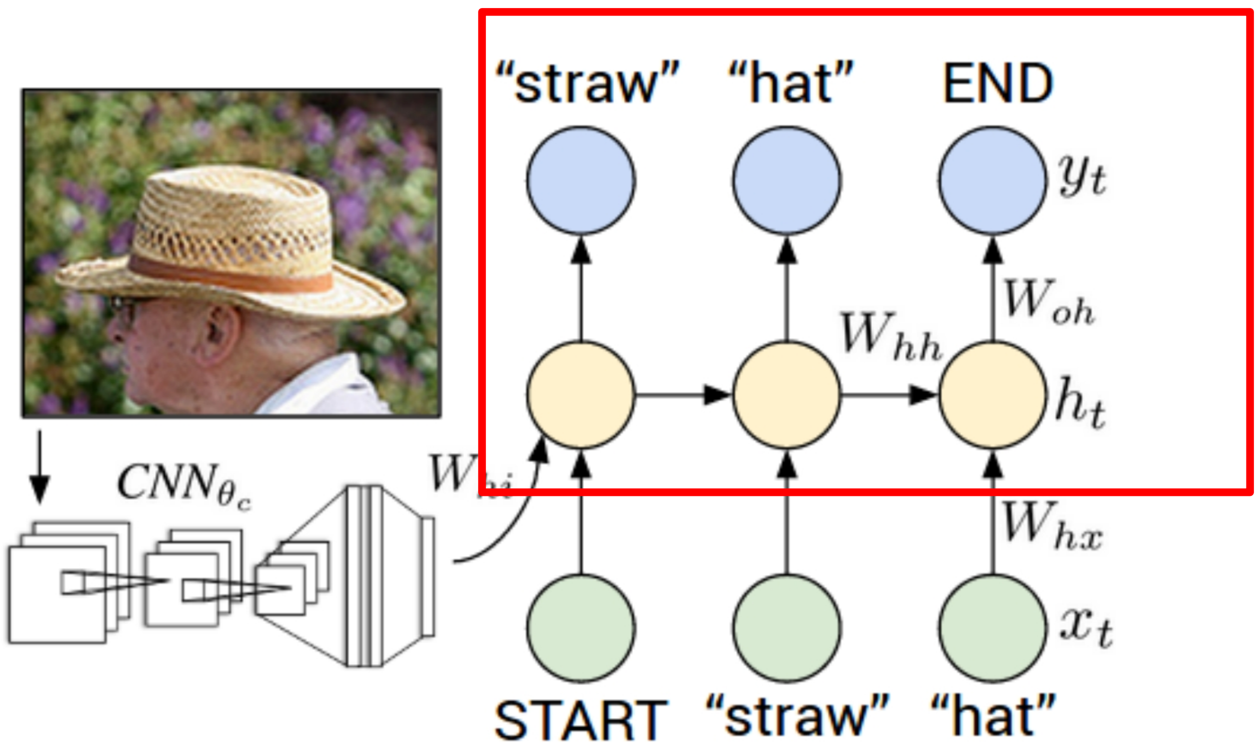


Image captioning with encoder-decoder system

- Example output (Vinyals et al., CVPR 2015)

A person riding a motorcycle on a dirt road.

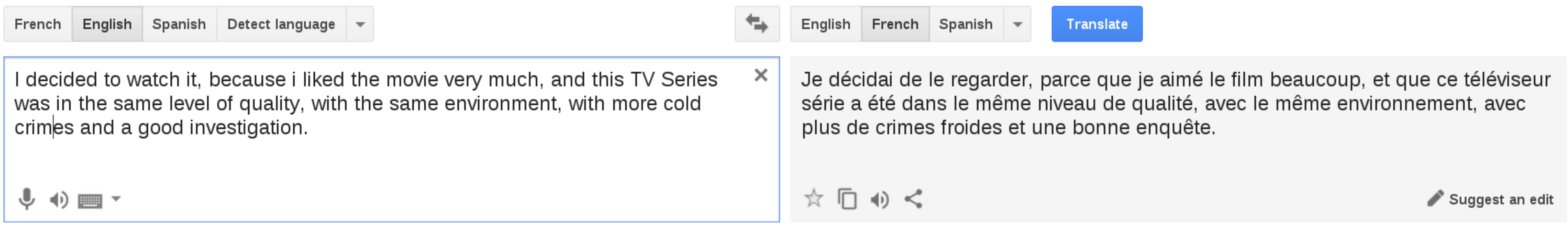
Two dogs play in the grass.

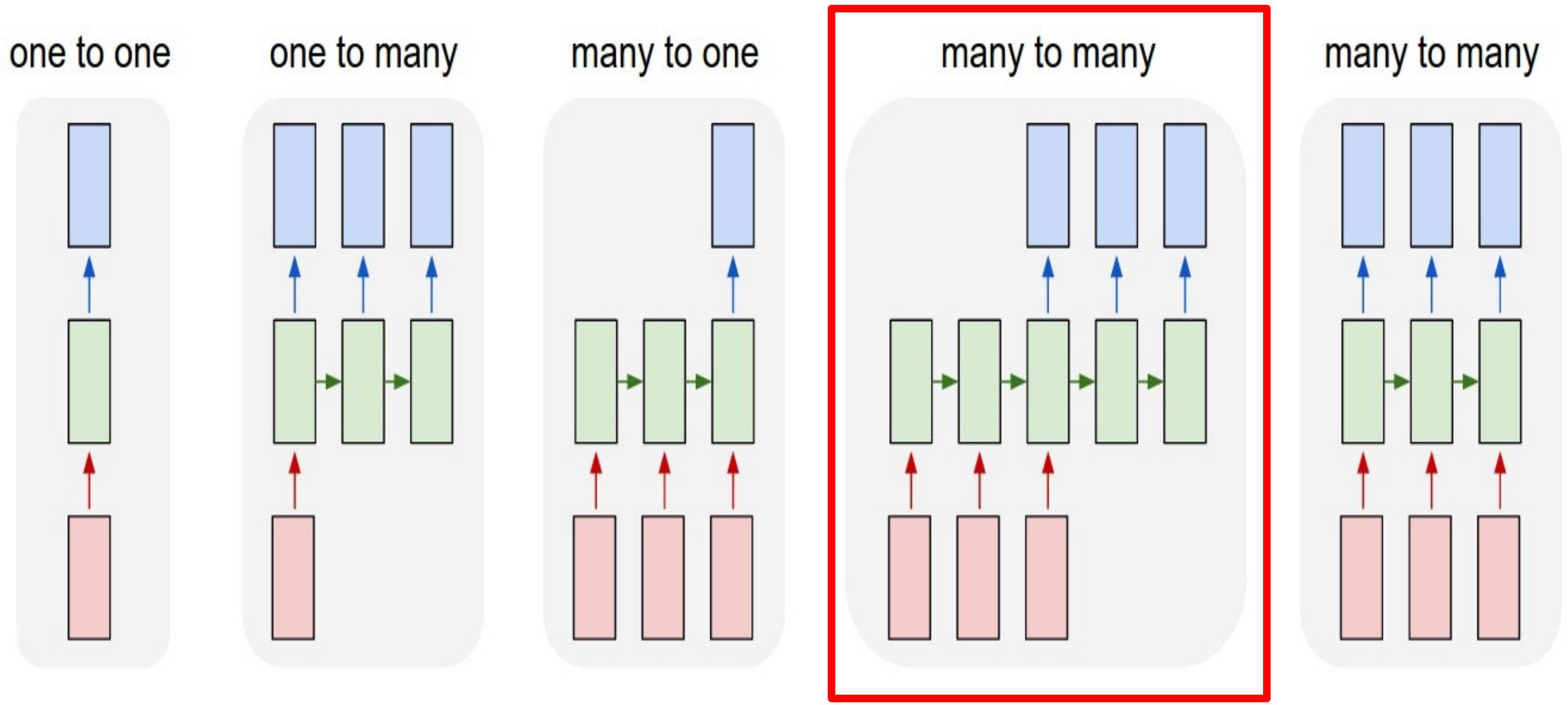
A group of young people playing a game of frisbee.

Two hockey players are fighting over the puck.

Encoder-decoder machine translation

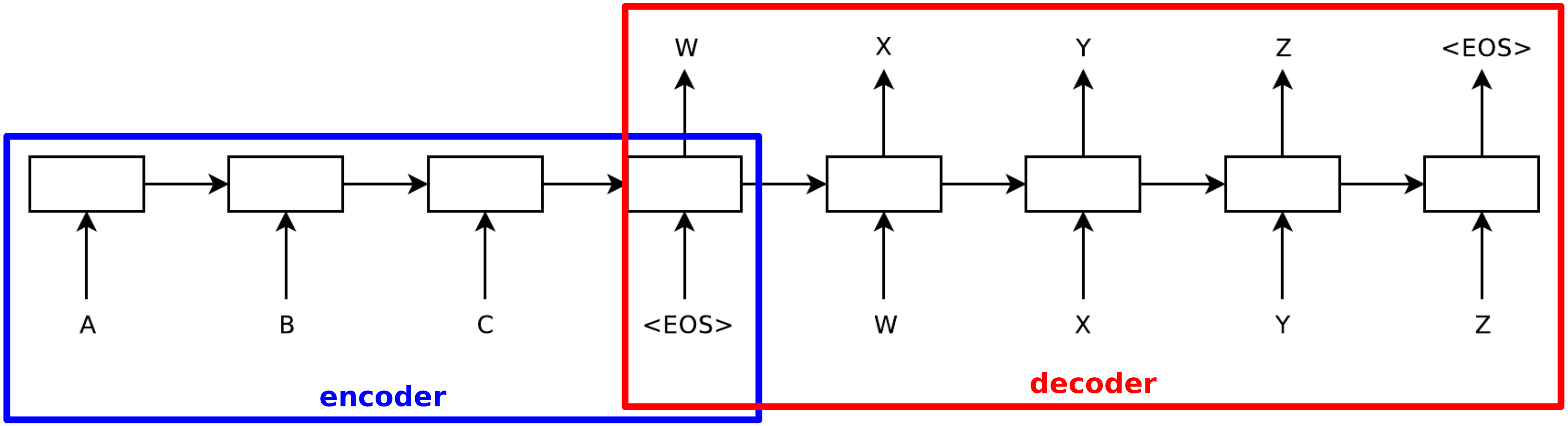
- Translation of a sentence into another language
  - Input and output of different length





Encoder-decoder machine translation

- Read source sentence with **encoder** RNN (Sutskever et al., NIPS 2014)
  - Can use bidirectional RNN since input sequence is given
- Generate target sentence with **decoder** RNN
  - Uses a different set of parameters
  - Uses output feedback to ensure output coherency
- Meaning of source sentence encoded in the RNN state vector passed between encoder and decoder
  - For the captioning model, a CNN is used as an image encoder



Encoder-decoder machine translation

- Decoder learns word embedding matrix G for output feedback

$$z_{i+1} = \phi\left(W z_i + G u_i\right)$$

- Decoder learns word embedding matrix F for word probabilities via softmax normalization

$$p_i = \sigma\left(F z_i\right)$$

- Encoder learns a word embedding matrix E
- Columns contain word vector embedding

$$s_i = E w_i$$

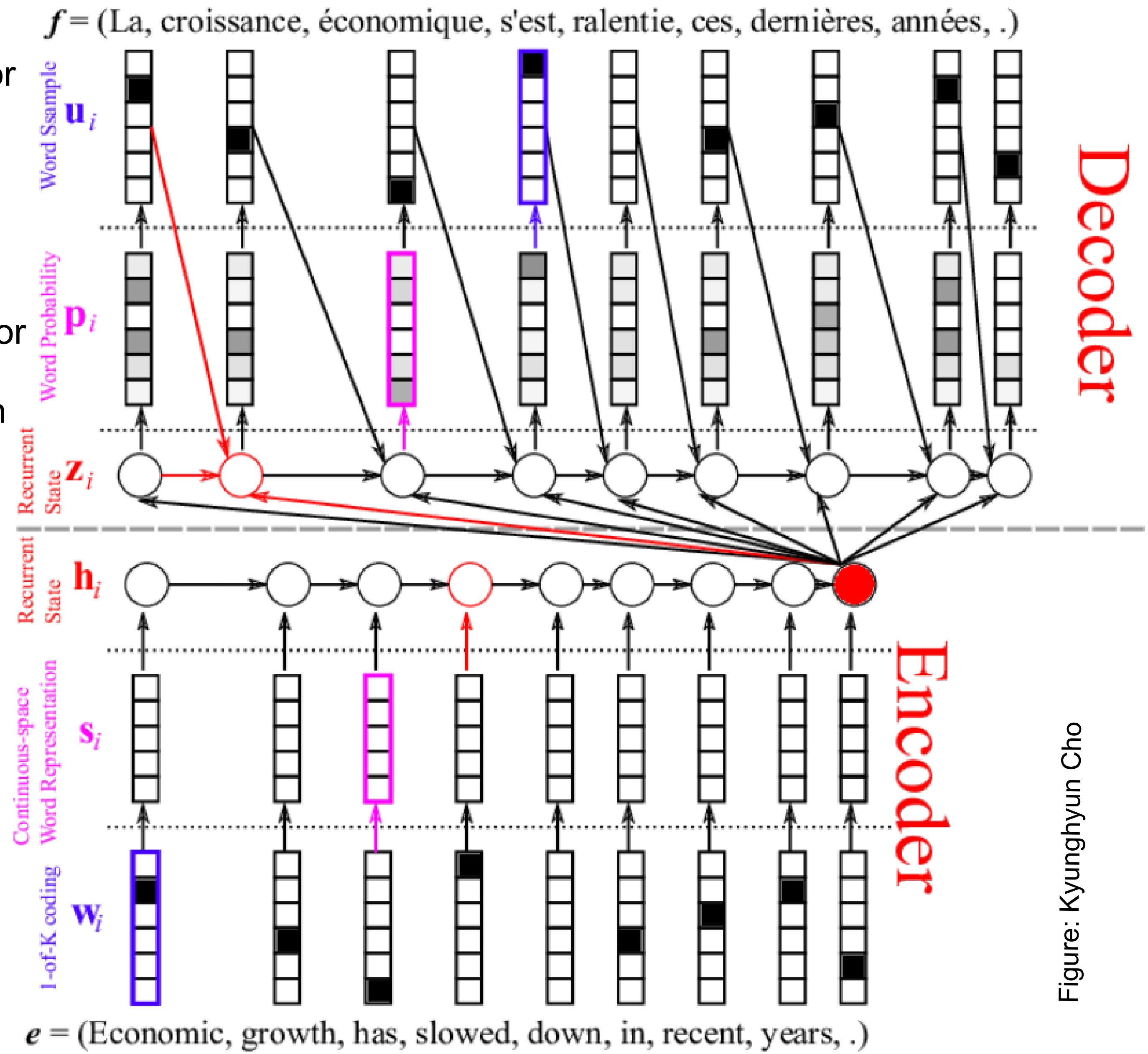
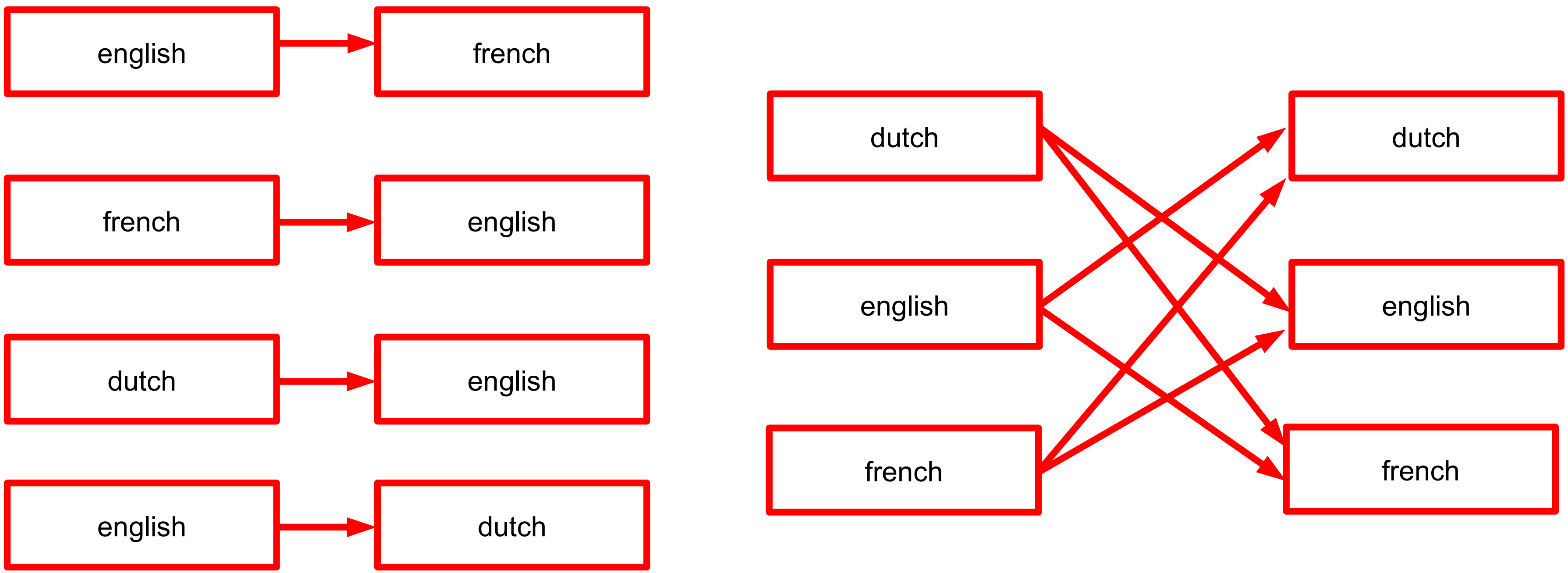


Figure: Kyunghyun Cho

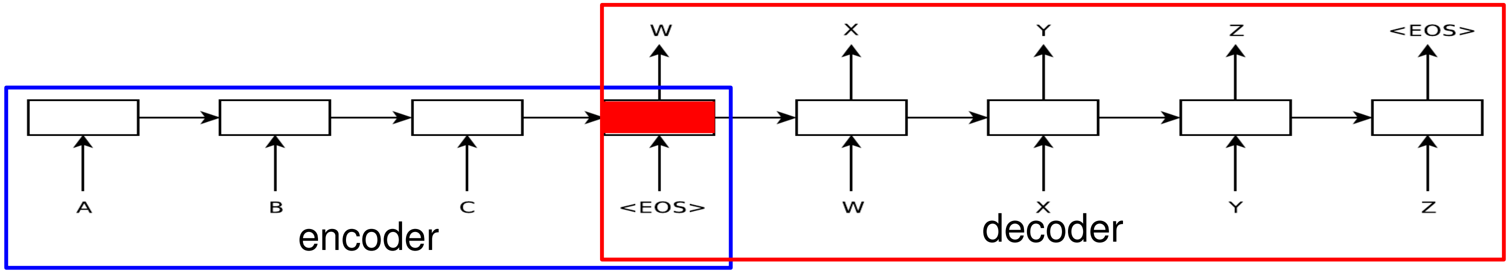
Encoder-decoder machine translation

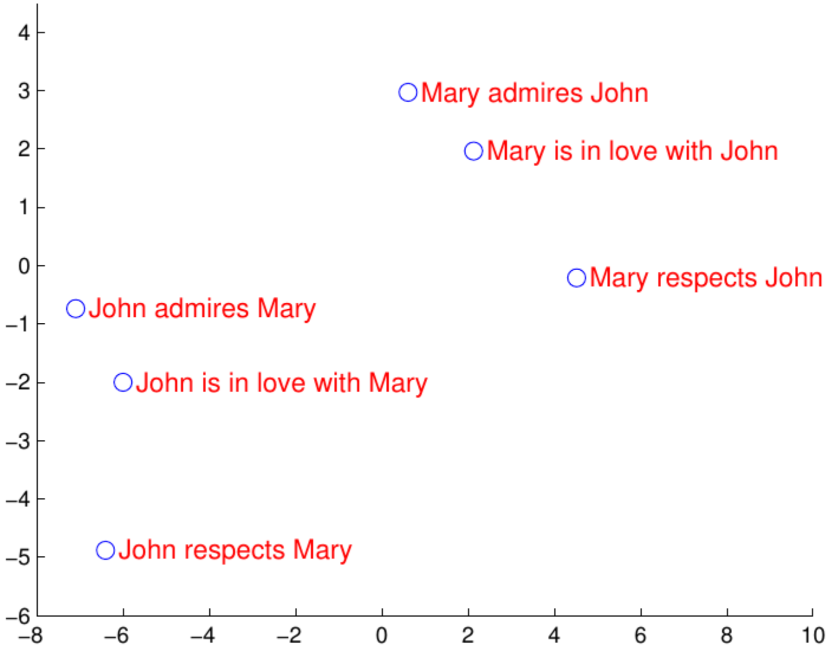
- Trained from “aligned” corpus of matching source-target sentences
- Encoder and decoder can be learned on multiple language pairs in parallel
  - (English to French) and (Dutch to French) use same decoder
  - (English to French) and (English to Dutch) use same encoder
- Generalizes to translation between new language pairs for which no aligned training corpus was available



Encoder-decoder machine translation

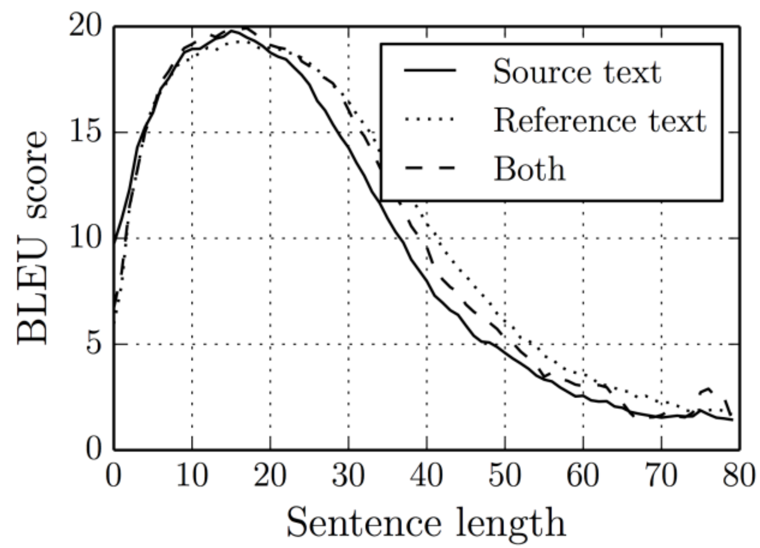
- PCA projection of LSTM encoder state after reading a sentence
  - Word order important for meaning, captured in encoder state vector



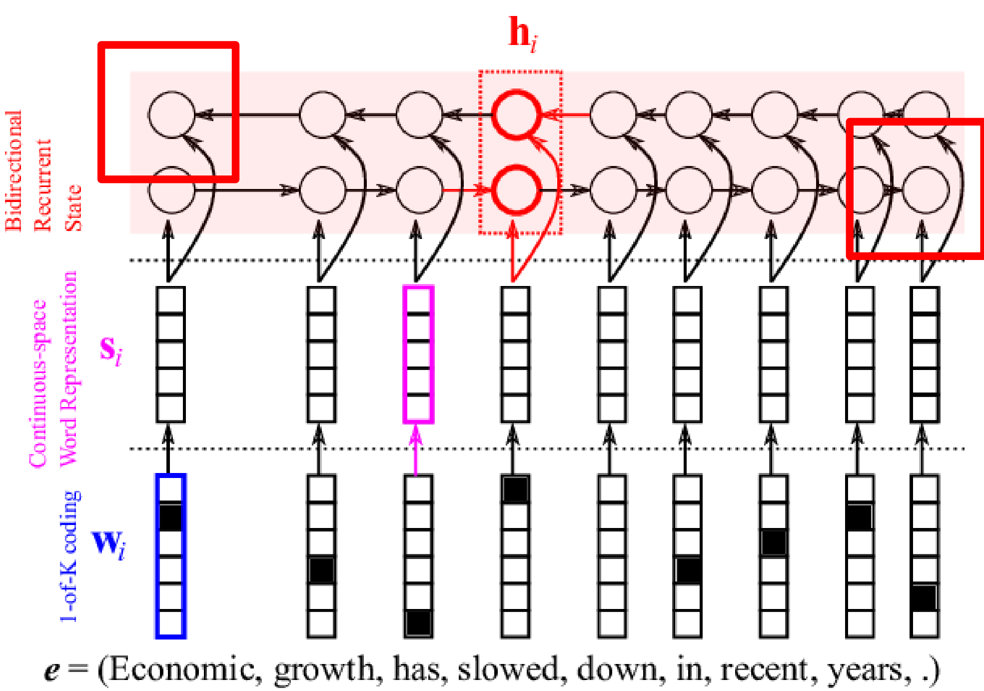


Attention mechanisms in RNNs

- Encoder-decoder based models compress the entire input into a single vector
  - Difficult to store all details as the sentences grow longer



- Sequential nature of RNN updates makes that start of sentence is less well encoded into the RNN state
  - Using bi-directional RNN helps, but not in the middle of the sentence...



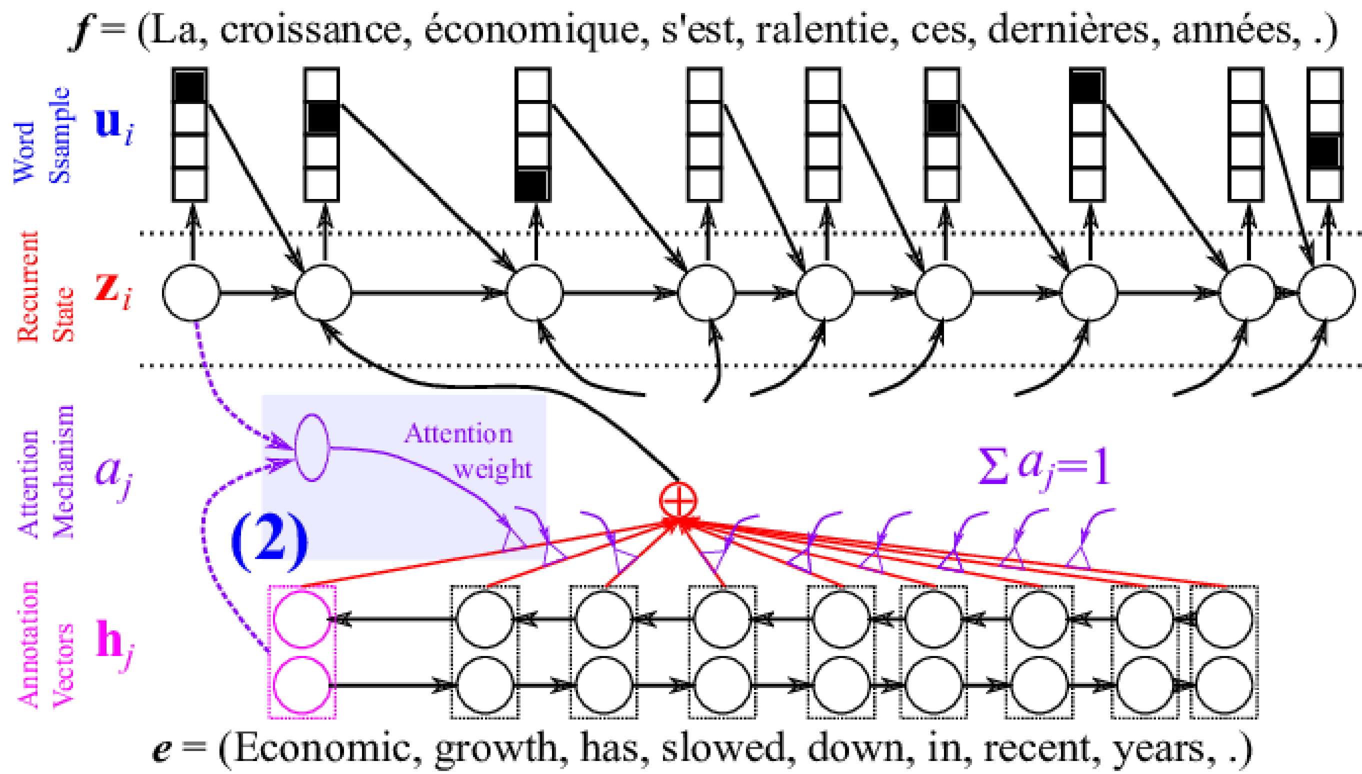
Attention mechanisms in RNNs

- Let decoder attend to part of the input for each state update
  - Selectively: based on current state and input representation
  - Should work for input sequences of variable size
- Sub-network takes state and input encoding, computes attention weights
  - Soft-max over candidate positions in the input
- Feed weighted sum of inputs to the state update

$$a_{ij} = \sigma(z_i, h_j)$$

$$c_i = \sum_{j=1}^{T} a_{ij} h_j$$

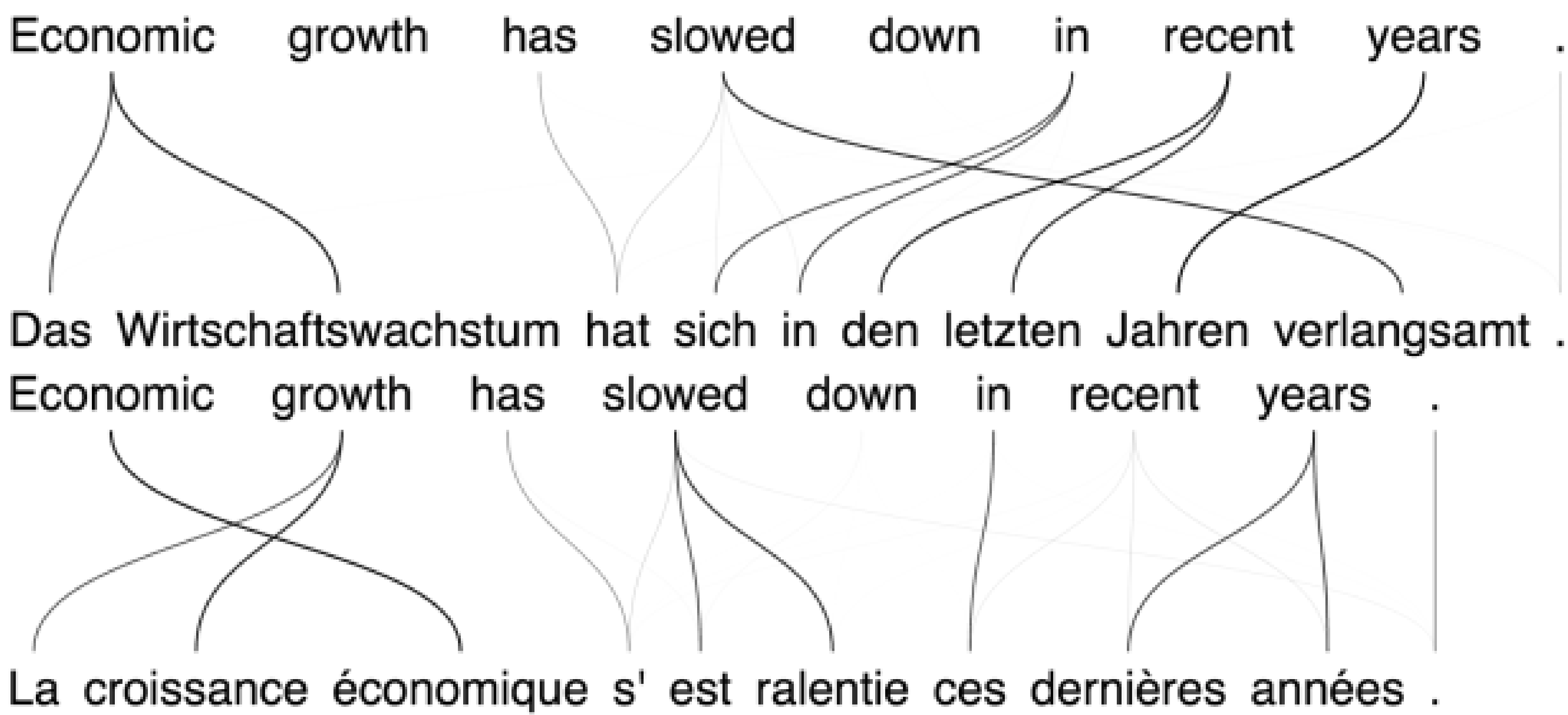
$$z_{i+1} = \phi(z_i, c_i, u_i)$$



[Bahdanau et al., ICLR'15]

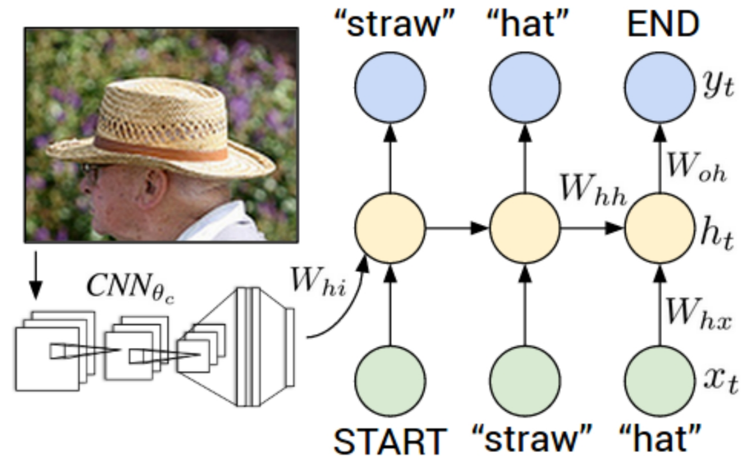
Attention mechanisms in RNNs

- Example correspondences identified by attention mechanism
  - Trained from sentence-level supervision, no word correspondences



Attention mechanisms in image captioning

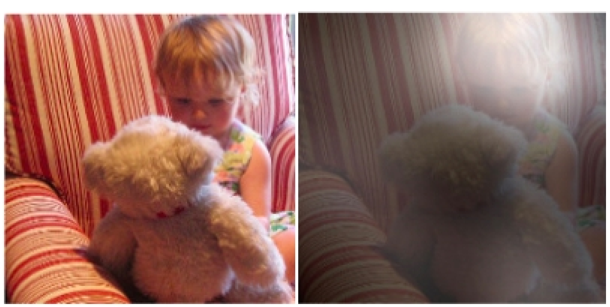
- Without attention image content encoded into vector output of CNN
  - Decoder cannot “look back” at image
- Attention can be used to focus decoder model on parts of input [Xu et al, ICML’15]



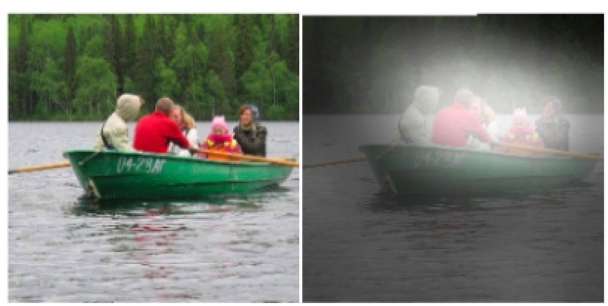
A woman is throwing a <u>frisbee</u> in a park.

A <u>dog</u> is standing on a hardwood floor.

A <u>stop</u> sign is on a road with a mountain in the background.



A little <u>girl</u> sitting on a bed with a teddy bear.



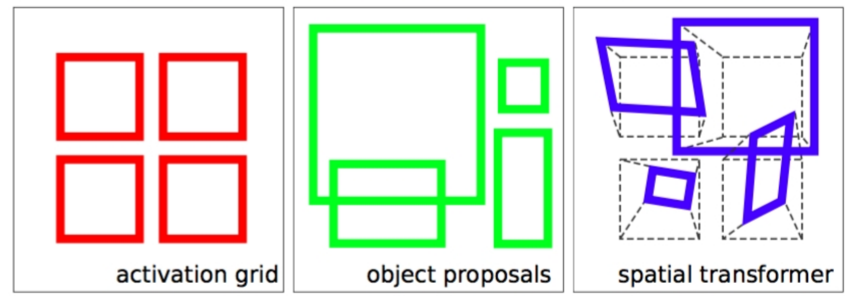
A group of <u>people</u> sitting on a boat in the water.

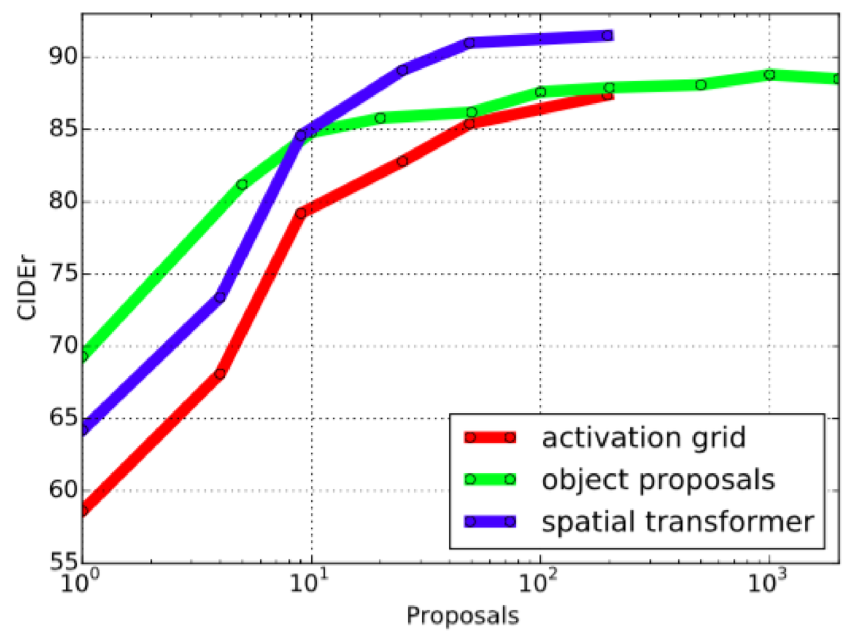
A giraffe standing in a forest with <u>trees</u> in the background.

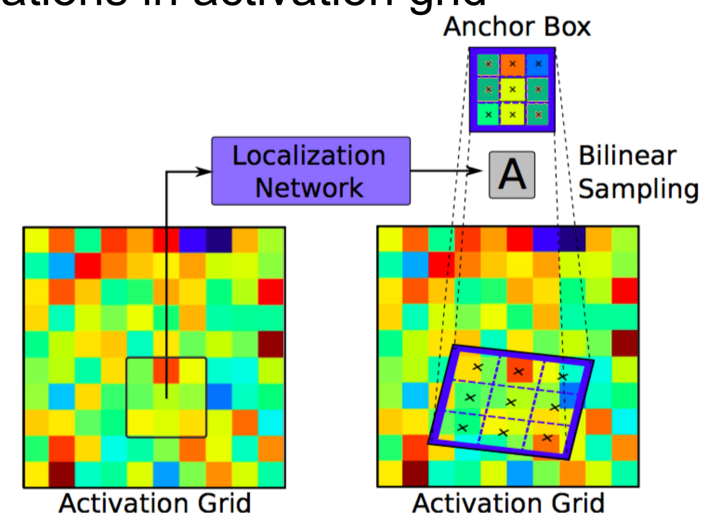
Attention mechanisms in image captioning

- What are the image “parts” that we should be looking at?
[Pedersoli et al, ICCV’17]
- Activation grid: the locations in a convolutional CNN layer
- Object proposals: plausible object locations predicted by external method
- Spatial transformer: regress deformation of default boxes at locations in activation grid

A **man** is flying a **kite** on a sandy **beach**.

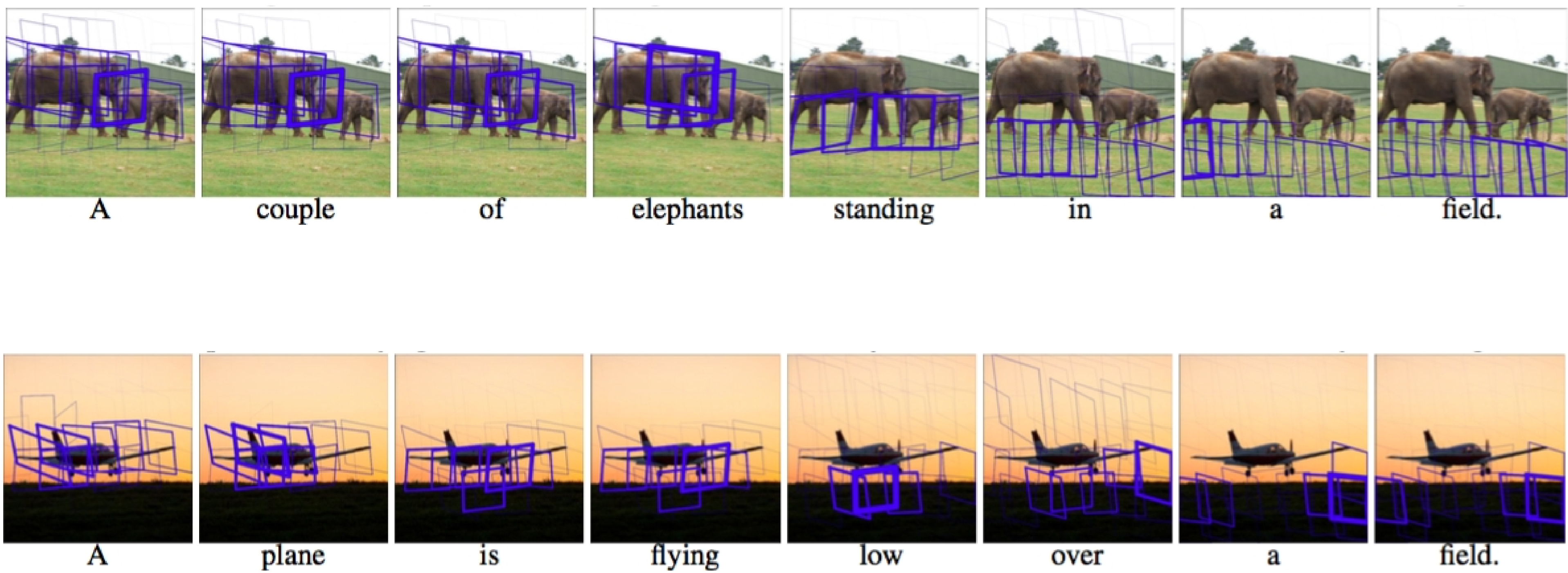






Attention mechanisms in image captioning

- Examples of generated sentences together with the attention regions
  - Region width proportional to attention weight [Pedersoli et al., ICCV'17]



Further reading

- "Pattern Recognition and Machine Learning"

  Chris Bishop.

  Springer, 2006.

- "Supervised Sequence Labelling with Recurrent Neural Networks"

  Alex Graves, 2012 (free online)

- "Deep Learning"

  Ian Goodfellow, Yoshua Bengio, Aaron Courville.

  MIT Press, in preparation.

  http://www.deeplearningbook.org/