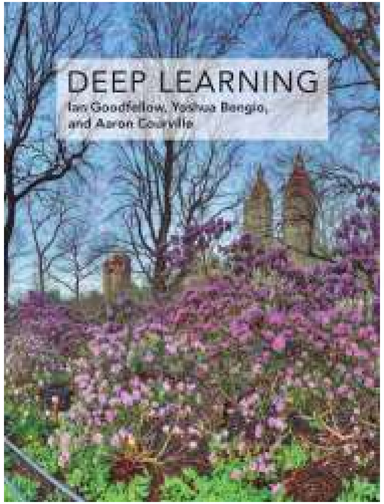
Recurrent Nets and Attention for System 2 Processing

Yoshua Bengio

July 30th, 2018, CIFAR Deep Learning & Reinforcement Learning Summer School, Toronto



Université de Mont

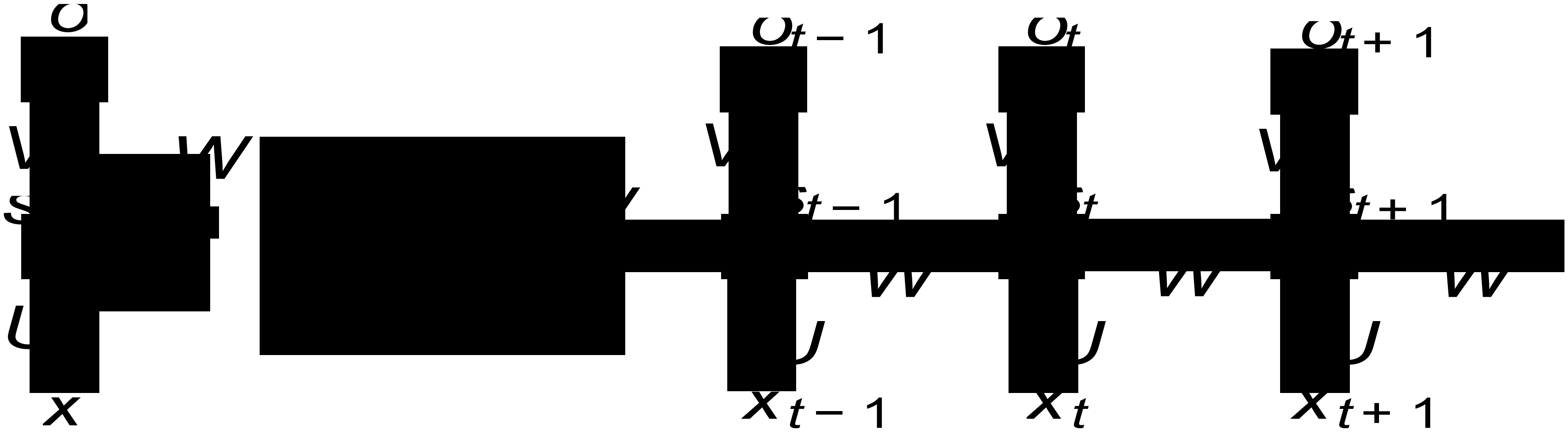
Mila

CIFAR | ICRA

CANADIAN INSTITUTE FOR ADVANCED RESEARCH | INSTITUT CANADIEN DE RECHERCHES AVANCÉES

Recurrent Neural Networks

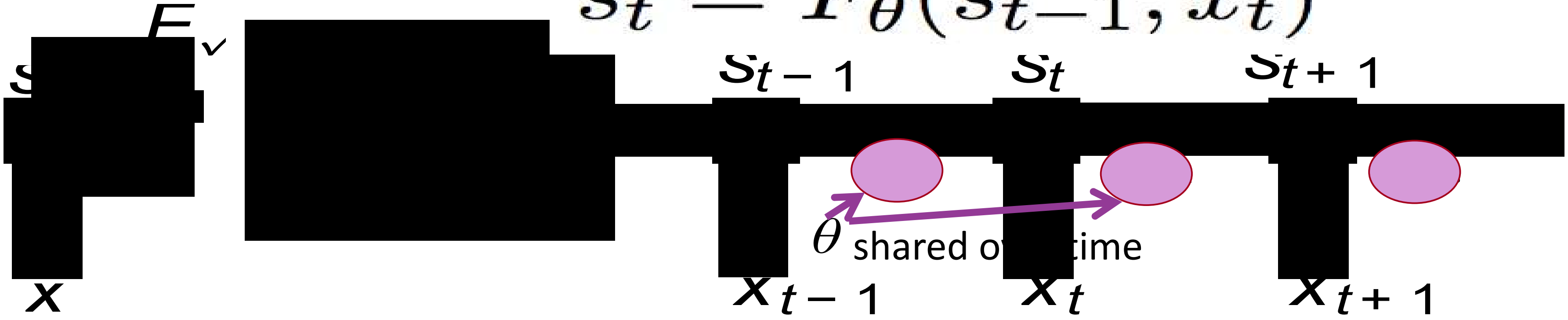
- Can read or produce an output at each time step: unfolding the graph tells us how to back-prop through time.



Recurrent Neural Networks

- Selectively summarize an input sequence in a fixed-size state vector via a recursive update

$$s_t = F_\theta(s_{t-1}, x_t)$$



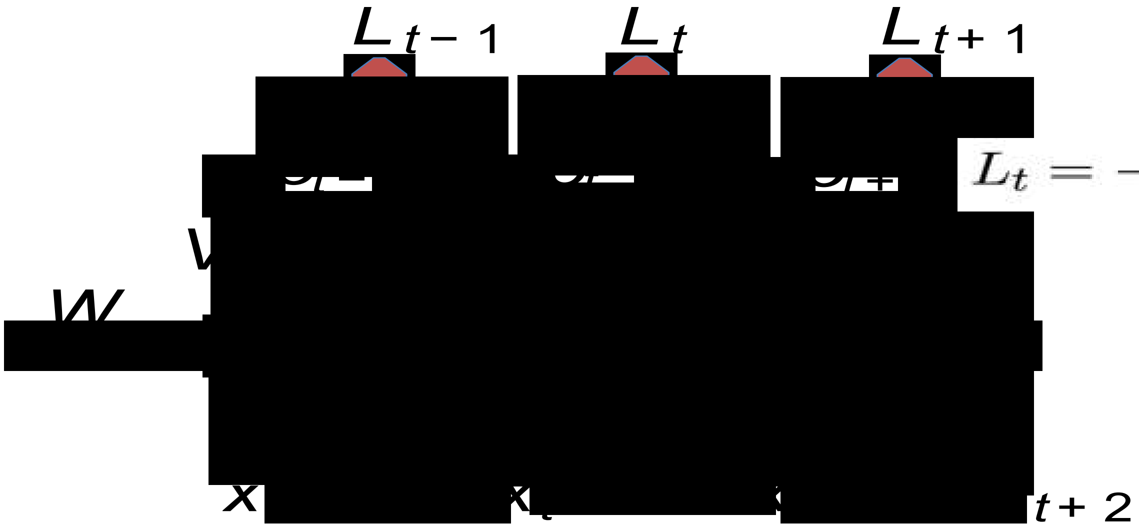
$$s_t = G_t(x_t, x_{t-1}, x_{t-2}, \ldots, x_2, x_1)$$

→ **Generalizes naturally to new lengths not seen during training**

Generative RNNs

- An RNN can represent a fully-connected **directed generative model**: every variable predicted from all previous ones.

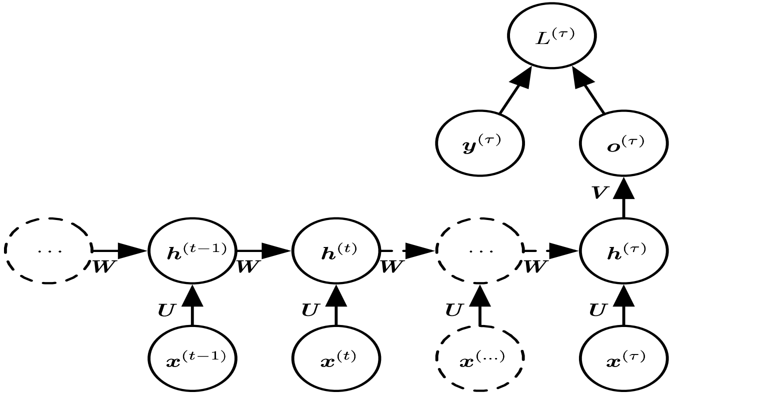
$$P(\mathbf{x}) = P(x_1, \ldots x_T) = \prod_{t=1}^{T} P(x_t | x_{t-1}, x_{t-2}, \ldots x_1)$$



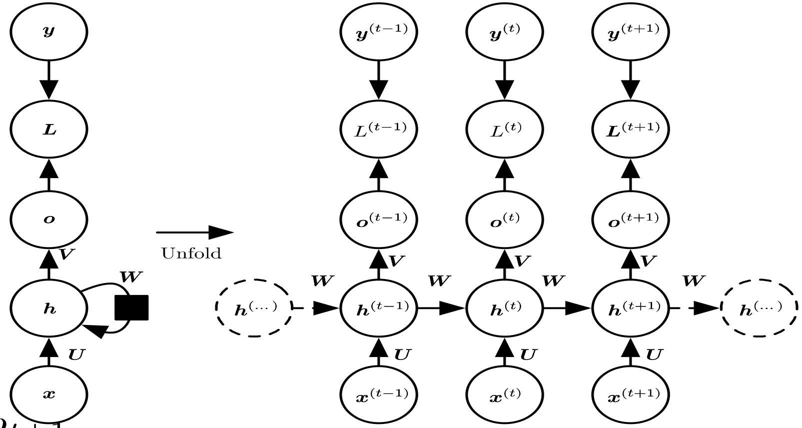
$$L_t = -\log P(x_t | x_{t-1}, x_{t-2}, \ldots x_1)$$

Conditional Distributions

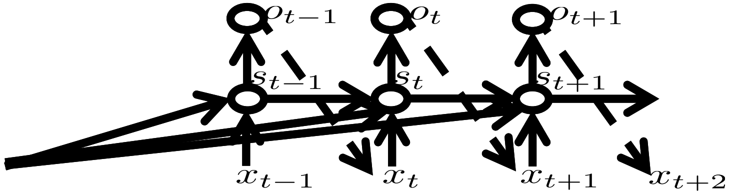
- Sequence to vector



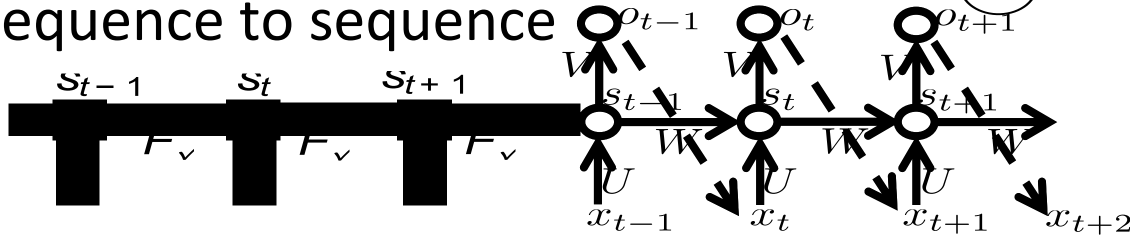
- Sequence to sequence of the same length, aligned



- Vector to sequence

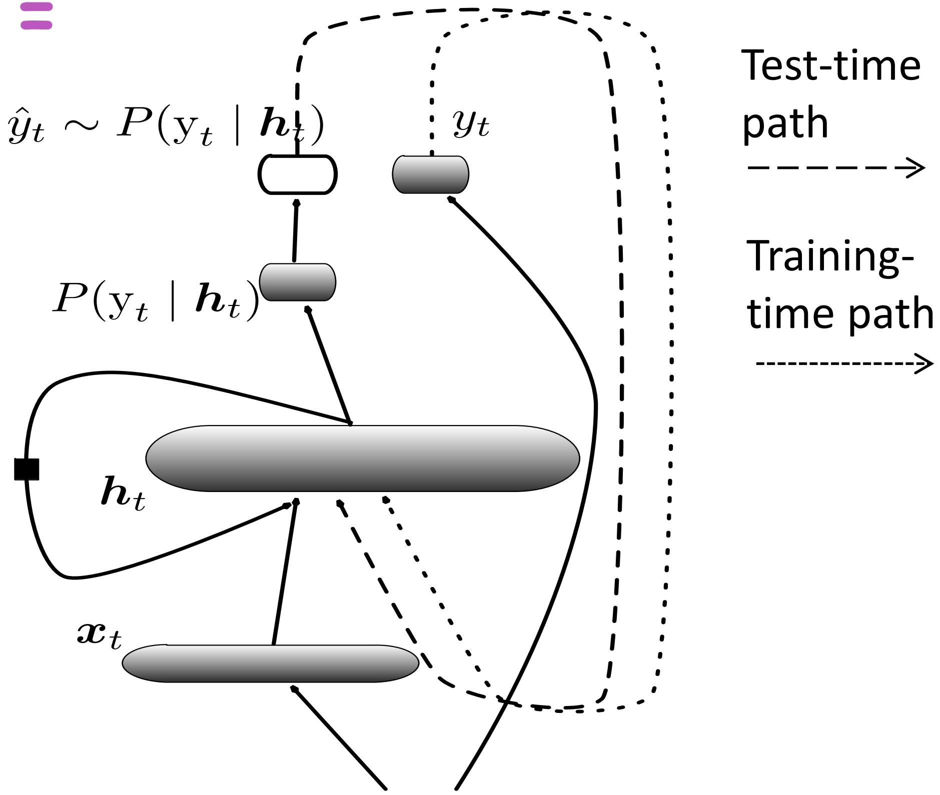


- Sequence to sequence



Maximum Likelihood = Teacher Forcing

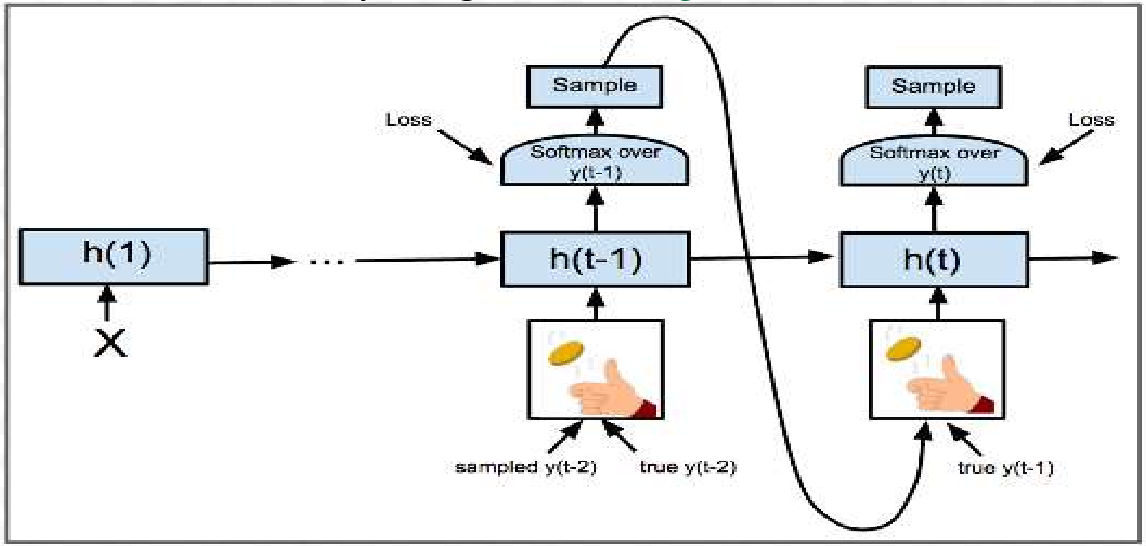
- During training, past *y* in input is from training data
- At generation time, past *y* in input is generated
- Mismatch can cause "compounding error"



$(\boldsymbol{x}_t, y_t)$: next input/output training pair

Ideas to reduce the train/generate mismatch in teacher forcing

- Scheduled sampling *(S. Bengio et al, NIPS 2015)*

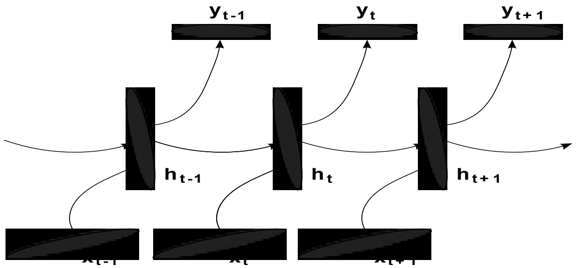


Related to
SEARN (Daumé et al 2009)
DAGGER (Ross et al 2010)
Gradually increase the probability of using the model's samples vs the ground truth as input.

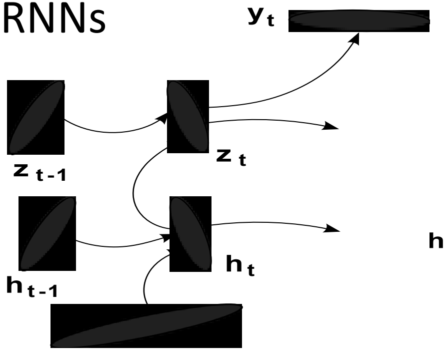
- Backprop through open-loop sampling recurrence & minimize long-term cost (but which one? GAN would be most natural → *Professor Forcing*, NIPS'2016)

Increasing the Expressive Power of RNNs with more Depth

- ICLR 2014, *How to construct deep recurrent neural networks*

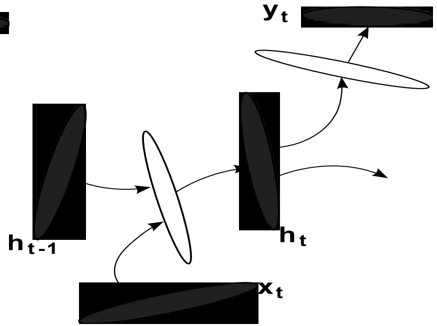


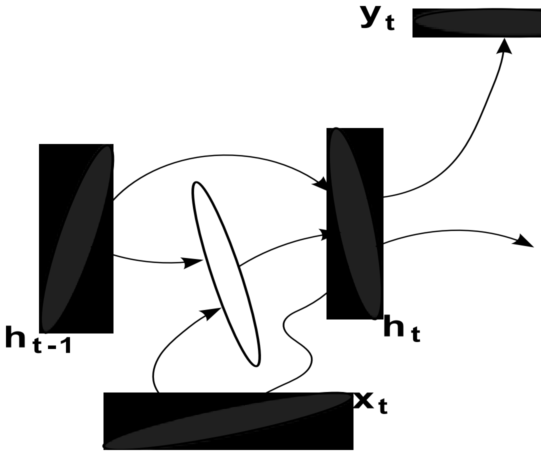
Ordinary RNNs



+ stacking

+ deep hid-to-out
+ deep hid-to-hid
+deep in-to-hid

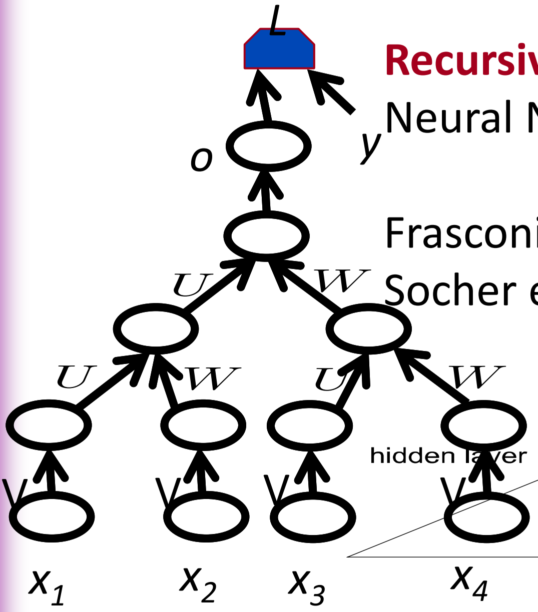




+ skip connections for creating shorter paths

Bidirectional RNNs, Recursive Nets, Multidimensional RNNs, etc.

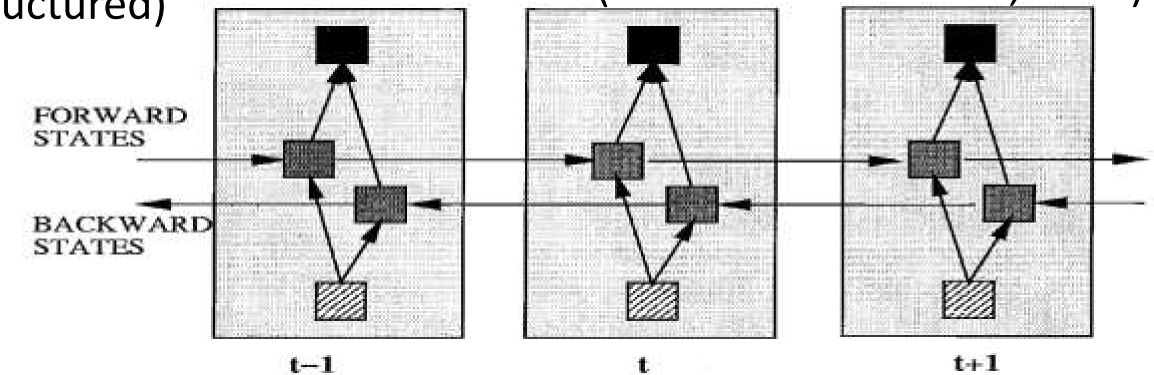
- The unfolded architecture needs not be a straight chain

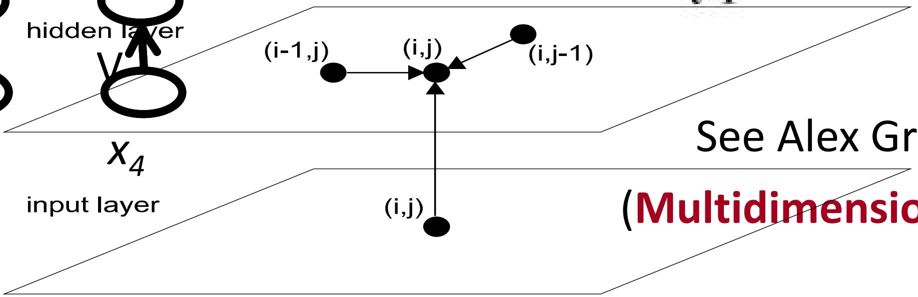


Recursive (tree-structured) Neural Nets:

Frasconi et al 97
Socher et al 2011

Bidirectional RNNs (Schuster and Paliwal, 1997)





See Alex Graves's work, e.g., 2012

(**Multidimensional** RNNs, Graves et al 2007)

Multiplicative Interactions

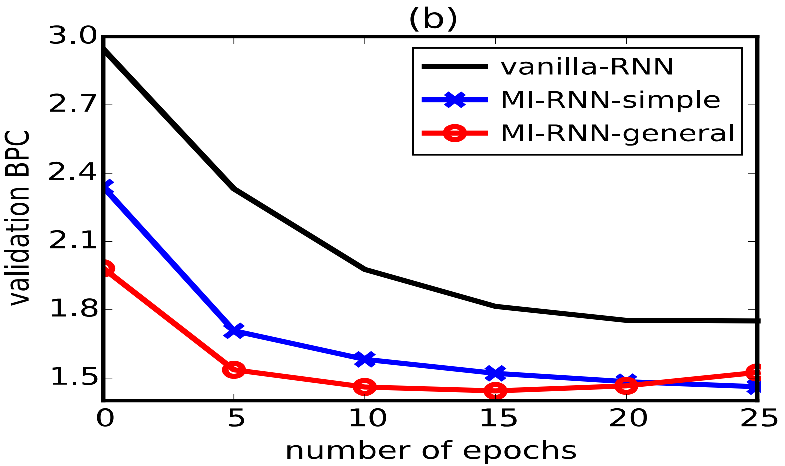
(Wu et al, 2016, arXiv:1606.06630)

- Multiplicative Integration RNNs:
  - Replace

$$\phi(\mathbf{W}\boldsymbol{x} + \mathbf{U}\boldsymbol{z} + \mathbf{b})$$

  - By

$$\phi(\mathbf{W}\boldsymbol{x} \odot \mathbf{U}\boldsymbol{z} + \mathbf{b})$$



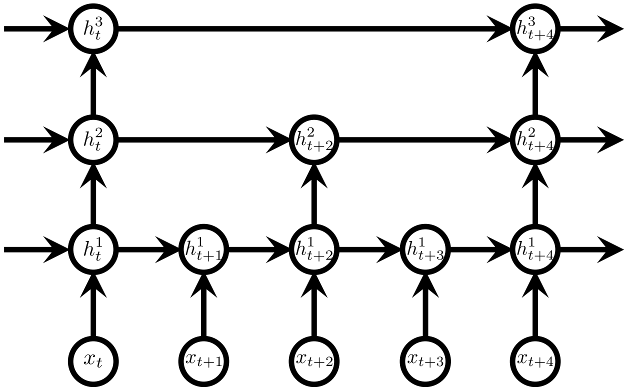
  - Or more general:

$$\phi(\boldsymbol{\alpha} \odot \mathbf{W}\boldsymbol{x} \odot \mathbf{U}\boldsymbol{z} + \boldsymbol{\beta}_1 \odot \mathbf{U}\boldsymbol{z} + \boldsymbol{\beta}_2 \odot \mathbf{W}\boldsymbol{x} + \boldsymbol{b})$$

Multiscale or Hierarchical RNNs

(Bengio & Elhihi, NIPS 1995)

- Motivation :
  - Gradients can propagate over longer spans through slow time-scale paths
- Approach :
  - Introduce a network architecture that update the states of its hidden layers with different speeds in order to capture multiscale representation of sequences.



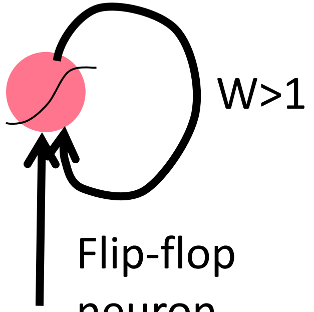
Learning Long-Term Dependencies with Gradient Descent is Difficult

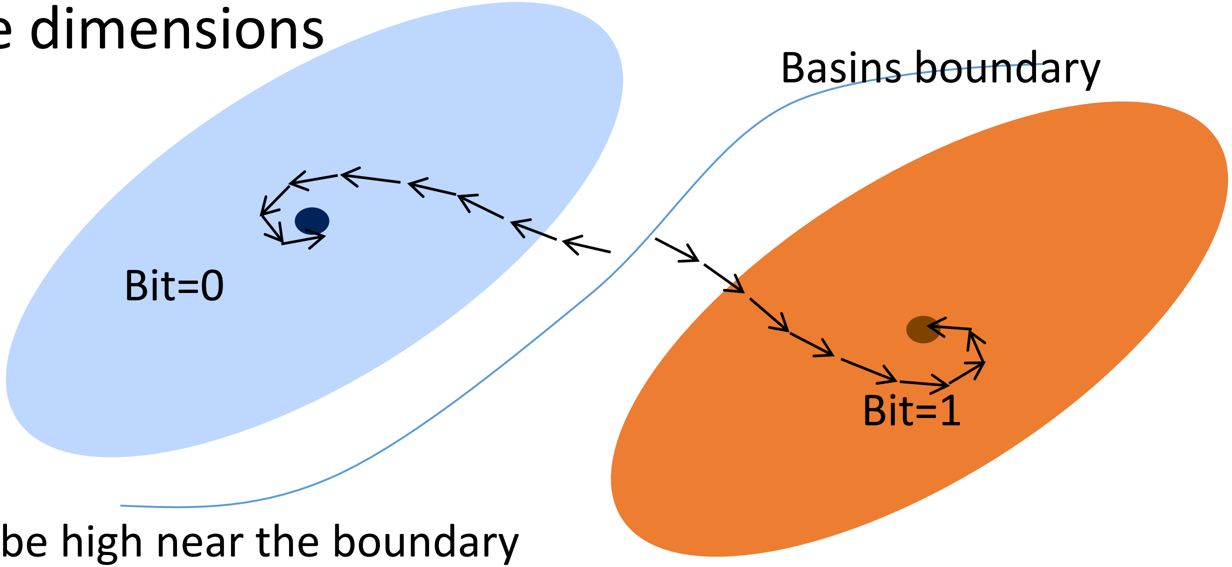


Y. Bengio, P. Simard & P. Frasconi, IEEE Trans. Neural Nets, **1994**

How to store 1 bit? Dynamics with multiple basins of attraction in some dimensions

- Some subspace of the state can store 1 or more bits of information if the dynamical system has multiple basins of attraction in some dimensions

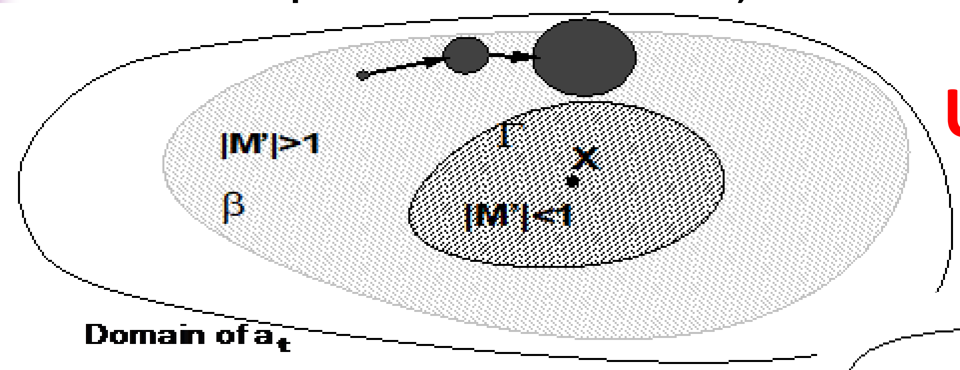




Note: gradients MUST be high near the boundary

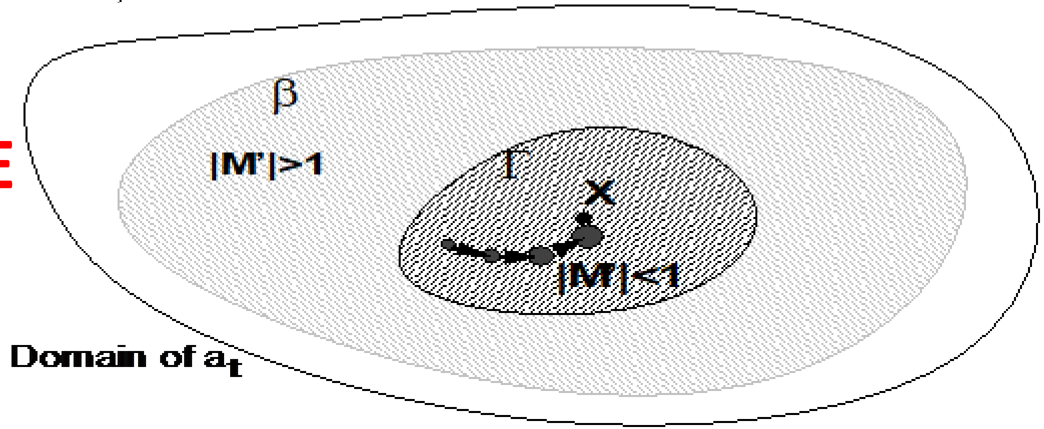
Robustly storing 1 bit in the presence of bounded noise

- With spectral radius > 1, noise can kick state out of attractor



UNSTABLE

CONTRACTIVE → STABLE



- Stable with radius<1

Storing Reliably ➔ Vanishing gradients

- Reliably storing bits of information requires spectral radius<1
- The product of T matrices whose spectral radius is < 1 is a matrix whose spectral radius converges to 0 at exponential rate in T

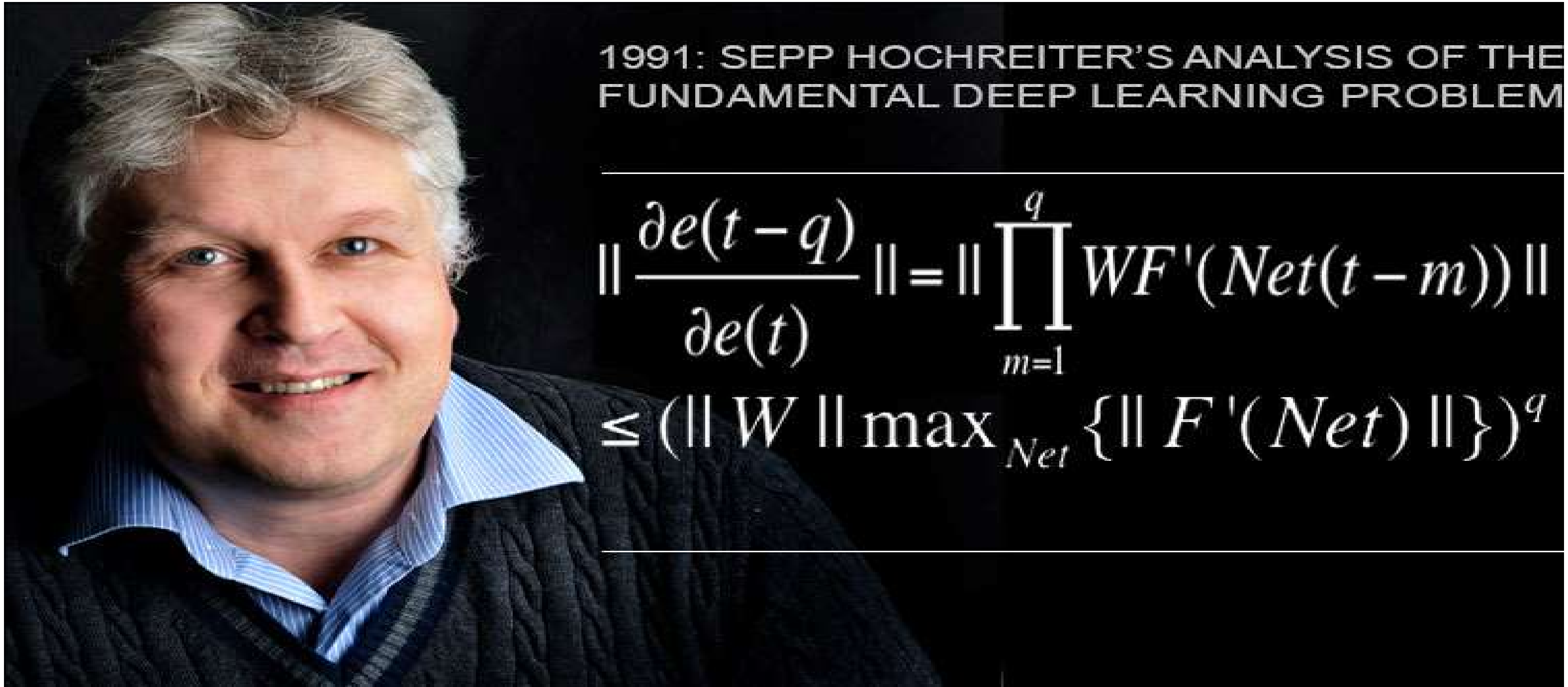
$$L = L(s_T(s_{T-1}(\ldots s_{t+1}(s_t, \ldots))))$$

$$\frac{\partial L}{\partial s_t} = \frac{\partial L}{\partial s_T} \frac{\partial s_T}{\partial s_{T-1}} \cdots \frac{\partial s_{t+1}}{\partial s_t}$$

- If spectral radius of Jacobian is < 1 ➔ propagated gradients vanish

Vanishing or Exploding Gradients

- Hochreiter's 1991 MSc thesis (in German) had independently discovered that backpropagated gradients in RNNs tend to either vanish or explode as sequence length increases



Why it hurts gradient-based learning

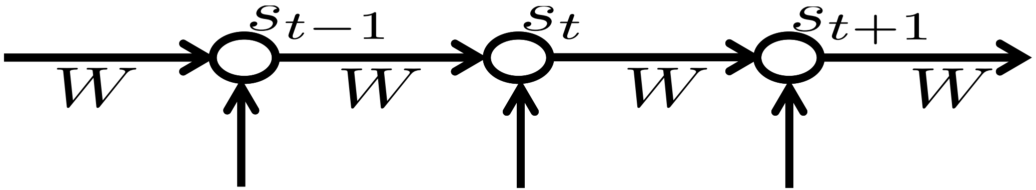
- Long-term dependencies get a weight that is exponentially smaller (in T) compared to short-term dependencies

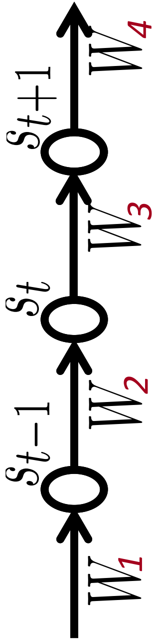
$$\frac{\partial C_t}{\partial W} = \sum_{\tau \leq t} \frac{\partial C_t}{\partial a_\tau} \frac{\partial a_\tau}{\partial W} = \sum_{\tau \leq t} \frac{\partial C_t}{\partial a_t} \text{[redacted]} \frac{\partial a_\tau}{\partial W}$$

Becomes exponentially smaller for longer time differences, when spectral radius < 1

Vanishing Gradients in Deep Nets are Different from the Case in RNNs

- If it was just a case of vanishing gradients in deep nets, we could just rescale the per-layer learning rate, but that does not really fix the training difficulties.





- Can't do that with RNNs because the weights are shared, & total true gradient = sum over different "depths"

$$\frac{\partial C_t}{\partial W} = \sum_{\tau \leq t} \frac{\partial C_t}{\partial a_\tau} \frac{\partial a_\tau}{\partial W} = \sum_{\tau \leq t} \frac{\partial C_t}{\partial a_t} \frac{\partial a_t}{\partial a_\tau} \frac{\partial a_\tau}{\partial W}$$

To store information robustly the dynamics must be contractive

- The RNN gradient is a product of Jacobian matrices, each associated with a step in the forward computation. To store information robustly in a finite-dimensional state, the dynamics must be contractive [Bengio et al 1994].

$$L = L(s_T(s_{T-1}(\ldots s_{t+1}(s_t, \ldots))))$$

$$\frac{\partial L}{\partial s_t} = \frac{\partial L}{\partial s_T} \frac{\partial s_T}{\partial s_{T-1}} \cdots \frac{\partial s_{t+1}}{\partial s_t}$$

Storing bits robustly requires e-values<1

- Problems:
  - e-values of Jacobians > 1 → *gradients explode*
  - **or e-values < 1 → *gradients shrink & vanish***
  - or random → variance grows exponentially

→ **Gradient clipping**

Dealing with Gradient Explosion by Gradient Norm Clipping

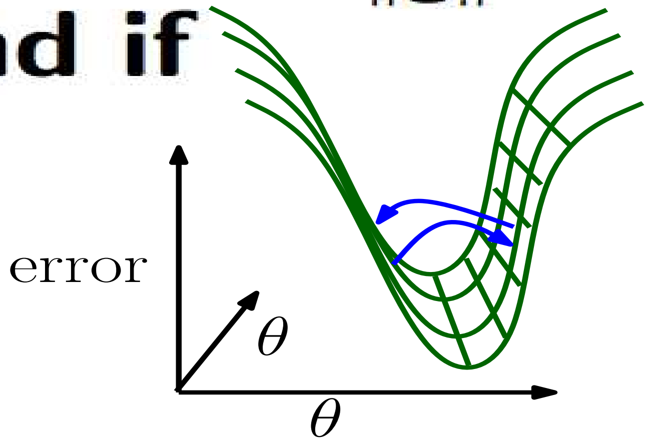
(Mikolov thesis 2012;
Pascanu, Mikolov, Bengio, ICML 2013)

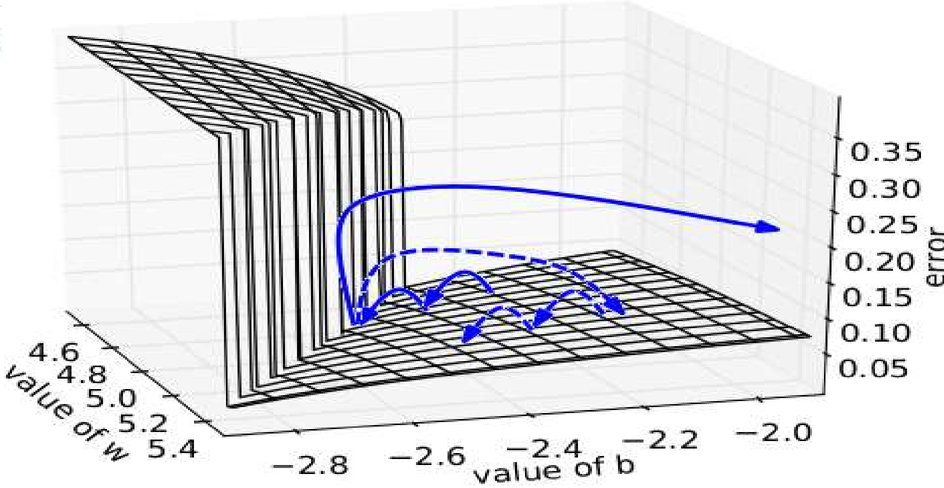
$$\hat{\mathbf{g}} \leftarrow \frac{\partial \mathit{error}}{\partial \theta}$$

if $\|\hat{\mathbf{g}}\| \geq \mathit{threshold}$ **then**

$$\hat{\mathbf{g}} \leftarrow \frac{\mathit{threshold}}{\|\hat{\mathbf{g}}\|}\hat{\mathbf{g}}$$

end if





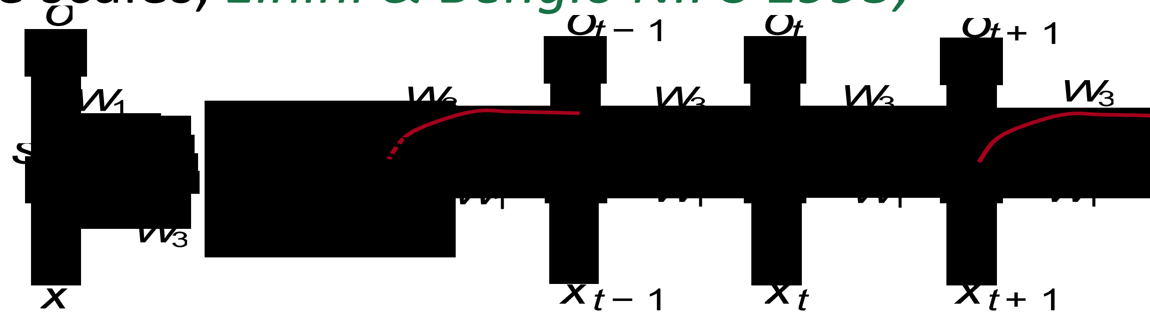
RNN Tricks

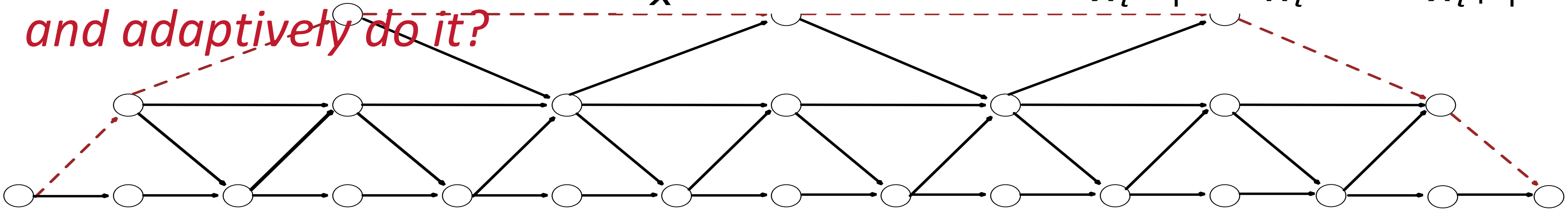
(Pascanu, Mikolov, Bengio, ICML 2013; Bengio, Boulanger & Pascanu, ICASSP 2013)

- Clipping gradients (avoid exploding gradients)
- Skip connections & leaky integration (propagate further)
- Multiple time scales / hierarchy (propagate further)
- Momentum (cheap 2nd order)
- Initialization (start in right ballpark avoids exploding/vanishing)
- Sparse Gradients (symmetry breaking)
- Gradient propagation regularizer (avoid vanishing gradient)
- Gated self-loops (LSTM & GRU, reduces vanishing gradient)

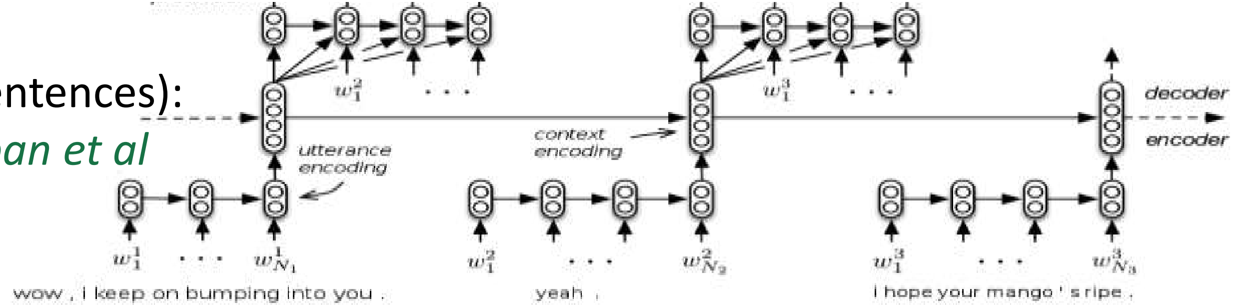
Delays & Hierarchies to Reach Farther

- Delays and multiple time scales, *Elhihi & Bengio NIPS 1995, Koutnik et al ICML 2014*
- *How to do this right?*
- *How to automatically and adaptively do it?*



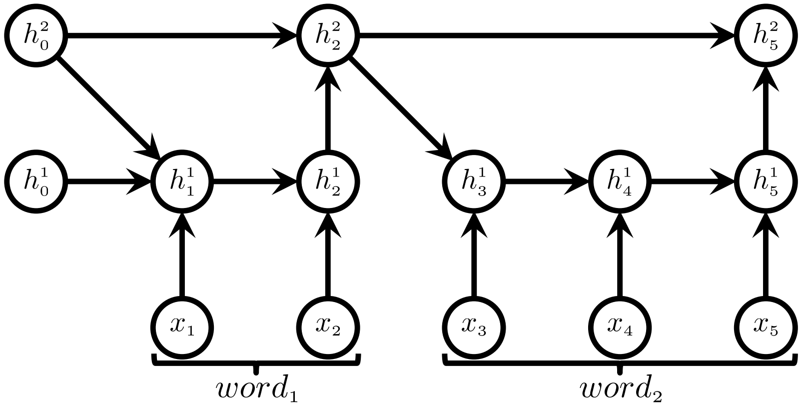


Hierarchical RNNs (words / sentences): *Sordoni et al CIKM 2015, Serban et al AAAI 2016*

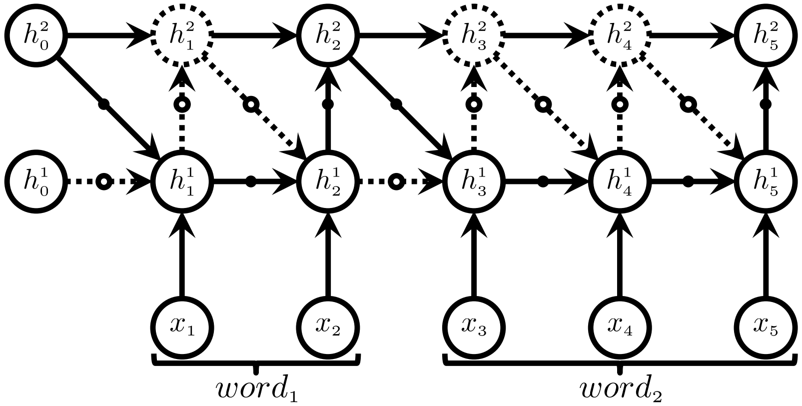


Multi-Scale: Chung, Cho & Bengio ACL'2016

Hand-crafted segmentation



Learned segmentation

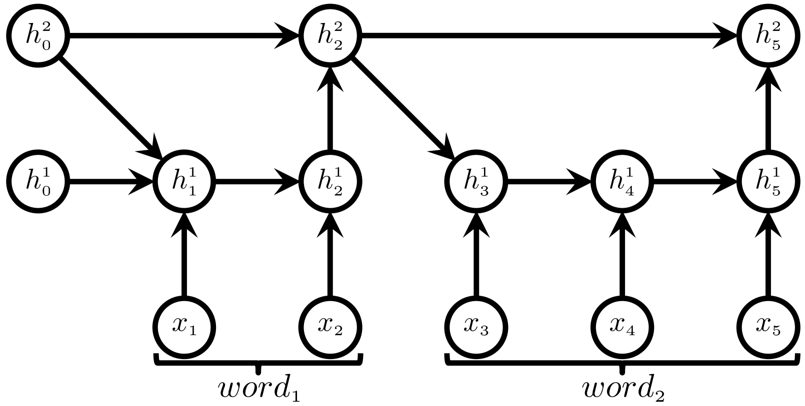


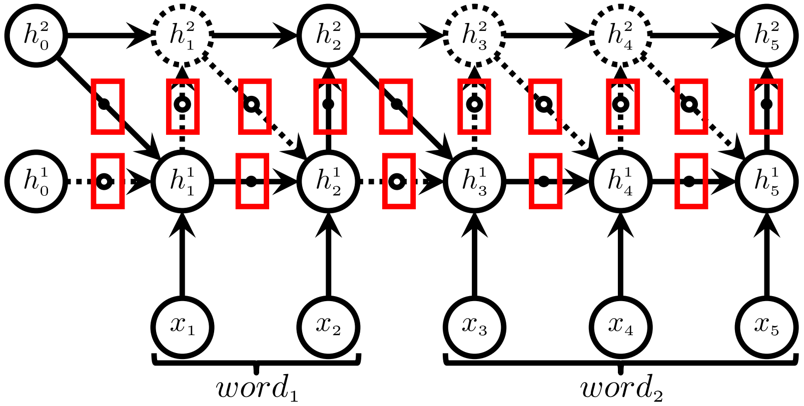
soft segmentation:
can be trained by backprop

Hierarchical Multiscale RNNs

Chung, Ahn & Bengio ICLR’2017

Boundary detectors have binary states!





Text8

Model	BPC
td-LSTM (Zhang et al., 2016)	1.63
HF-MRNN (Mikolov et al., 2012)	1.54
MI-RNN (Wu et al., 2016)	1.52
Skipping-RNN (Pachitariu & Sahani, 2013)	1.48
MI-LSTM (Wu et al., 2016)	1.44
BatchNorm LSTM (Cooijmans et al., 2016)	1.36
HM-LSTM	1.32
LayerNorm HM-LSTM	**1.29**

Gradient signal:

- straight-through
- REINFORCE

Fighting the vanishing gradient: LSTM & GRU

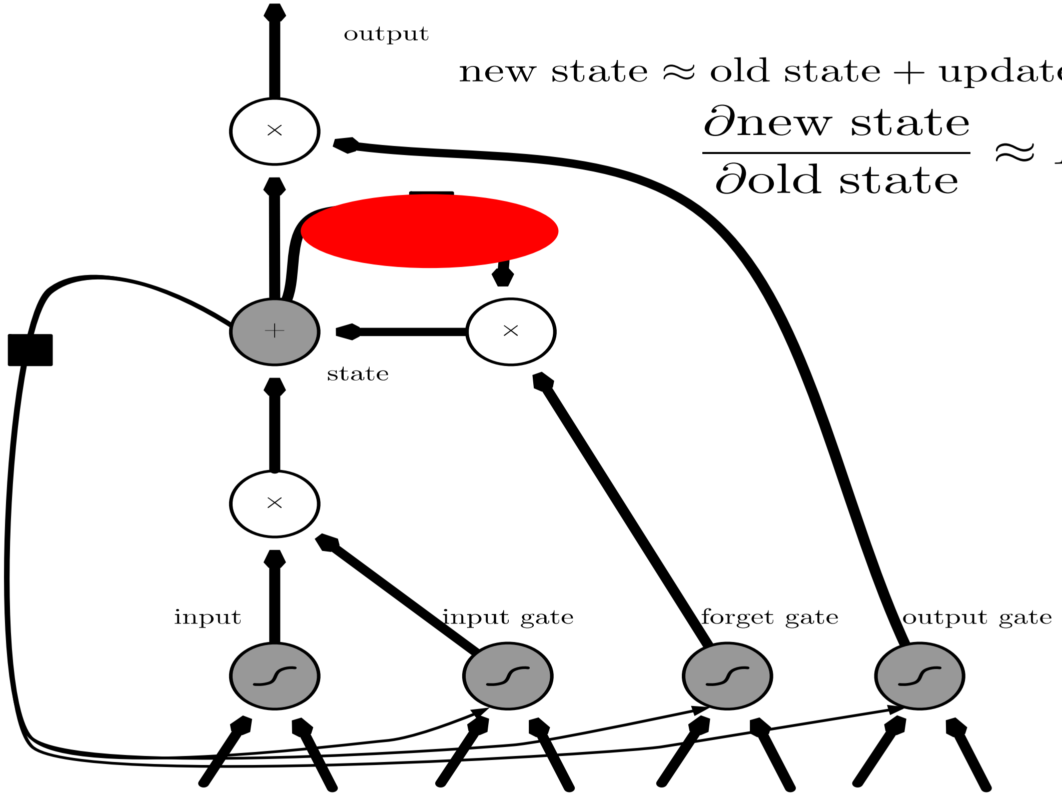
(Hochreiter 1991); first version of the LSTM, called Neural Long-Term Storage with self-loop

- Create a path where gradients can flow for longer with a
- Corresponds to an eigenvalue of Jacobian slightly less than 1
- LSTM is now **heavily used** *(Hochreiter & Schmidhuber 1997)*
- GRU light-weight version *(Cho et al 2014)*

LSTM: (Hochreiter & Schmidhuber 1997)

$$\text{new state} \approx \text{old state} + \text{update}$$

$$\frac{\partial \text{new state}}{\partial \text{old state}} \approx I$$



Gating for Attention-Based Neural Machine Translation

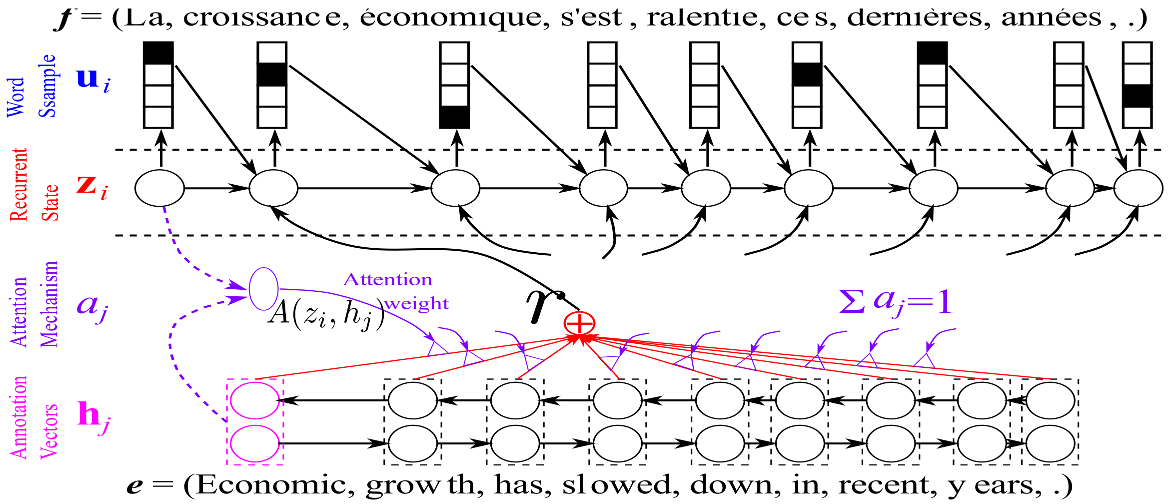
Related to earlier Graves 2013 for generating handwriting

- *(Bahdanau, Cho & Bengio, arXiv sept. 2014, ICLR 2015)*
- *(Jean, Cho, Memisevic & Bengio, arXiv dec. 2014, ACL 2015)*

$$a_j = \frac{e^{A(z_i, h_j)}}{\sum_{j'} e^{A(z_i, h_{j'})}}$$

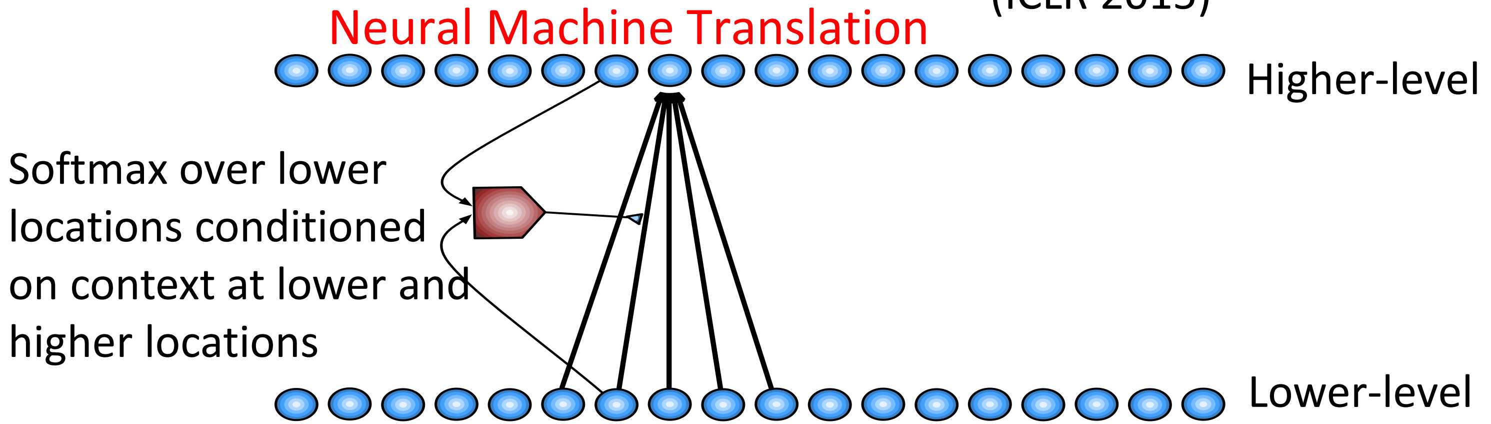
$$r = \sum_j a_j h_j$$

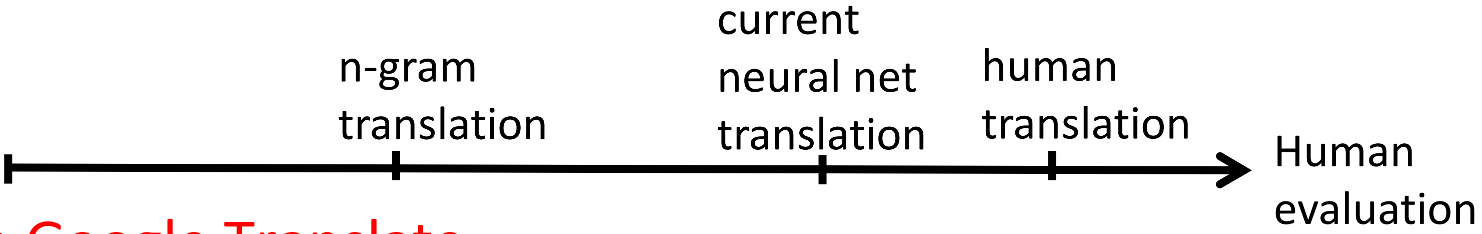
Read = weighted average of attended contents



Gating for Attention-Based Neural Machine Translation

- Incorporating the idea of **attention, using GATING units,** has unlocked a breakthrough in machine translation: (ICLR'2015)

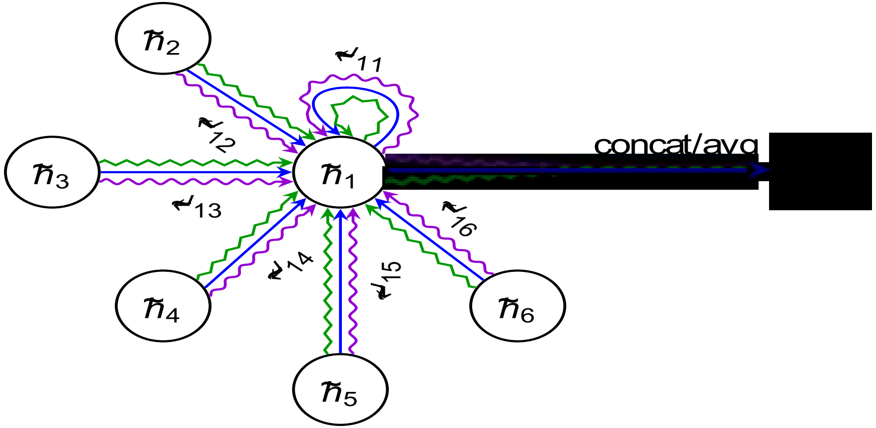




- Now in Google Translate

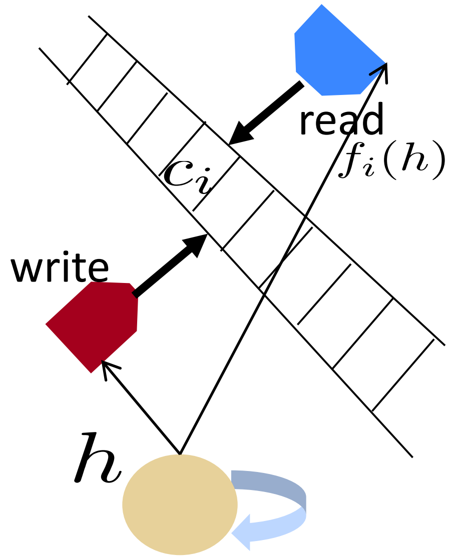
Graph Attention Networks
Velickovic et al, ICLR 2018

- Handle variable-size neighborhood of each node using the same neural net by using an attention mechanism to aggregate information from the neighbors
- Use multiple attention heads to collect different kinds of information



Attention Mechanisms for Memory Access

- Neural Turing Machines *(Graves et al 2014)*
- and Memory Networks *(Weston et al 2014)*
- Use a content-based attention mechanism *(Bahdanau et al 2014)* to control the read and write access into a memory
- The attention mechanism outputs a softmax over memory locations



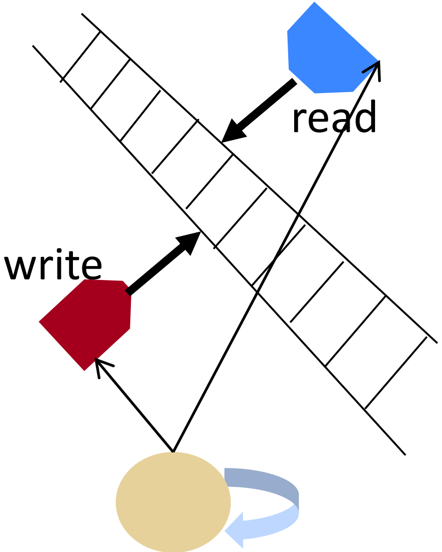
$$\alpha_i = \frac{e^{f_i(h)}}{\sum_j e^{f_j(h)}}$$

Read = weighted average of attended contents

$$r = \sum_i \alpha_i c_i$$

From Memory to System 2

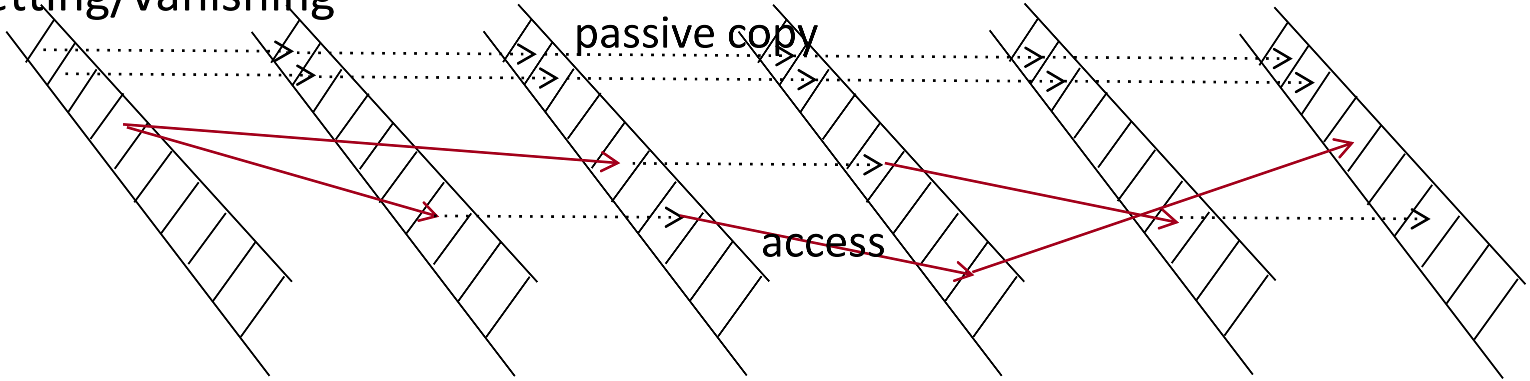
- Attention has also opened the door to neural nets which can write to and read from a memory
  - 2 systems:
    - Cortex-like (state controller and representations)
      - **System 1, intuition, fast heuristic answer (what current DL does quite well)**
    - Hippocampus-like (memory) + prefrontal cortex
      - System 2, slow, logical, sequential



- Memory-augmented networks gave rise to
  - Systems which reason
    - Sequentially combining several selected pieces of information (from the memory) in order to obtain a conclusion
  - Systems which answer questions
    - Accessing relevant facts and combining them

Large Memory Networks: Sparse Access Memory for Long-Term Dependencies

- Memory = part of the state
- Memory-based networks are special RNNs
- A mental state stored in an external memory can stay for arbitrarily long durations, until it is overwritten (partially or not)
- Forgetting = vanishing gradient.
- Memory = **higher-dimensional state**, avoiding or reducing the need for forgetting/vanishing

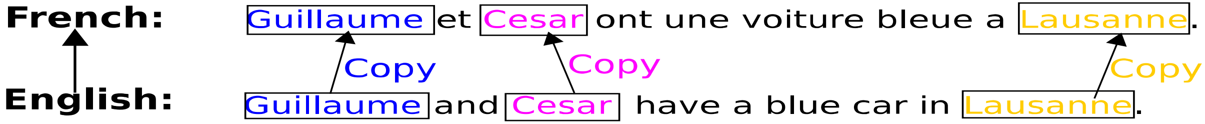


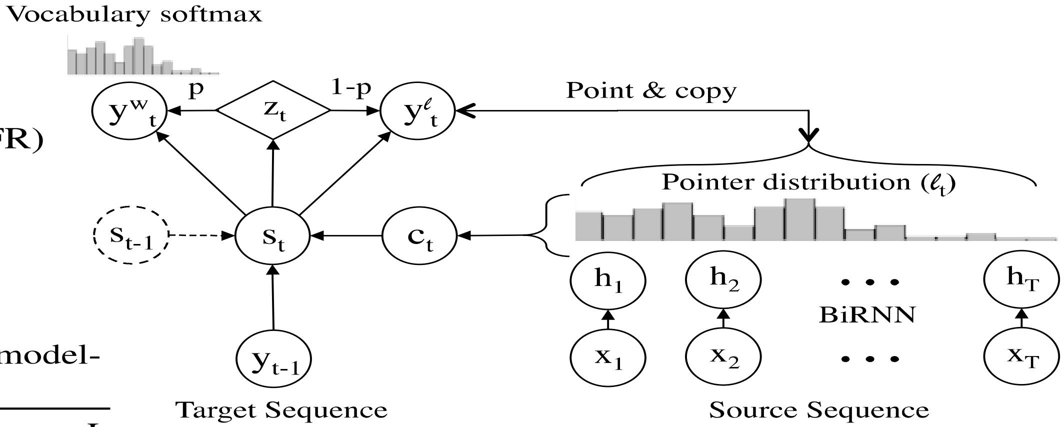
Pointing the Unknown Words

Gulcehre, Ahn, Nallapati, Zhou & Bengio ACL 2016

Based on 'Pointer Networks', Vinyals et al 2015

The next word generated can either come from vocabulary or is copied from the input sequence.





Machine Translation

Table 5: Europarl Dataset (EN-FR)

	BLEU-4
NMT	20.19
NMT + PS	**23.76**

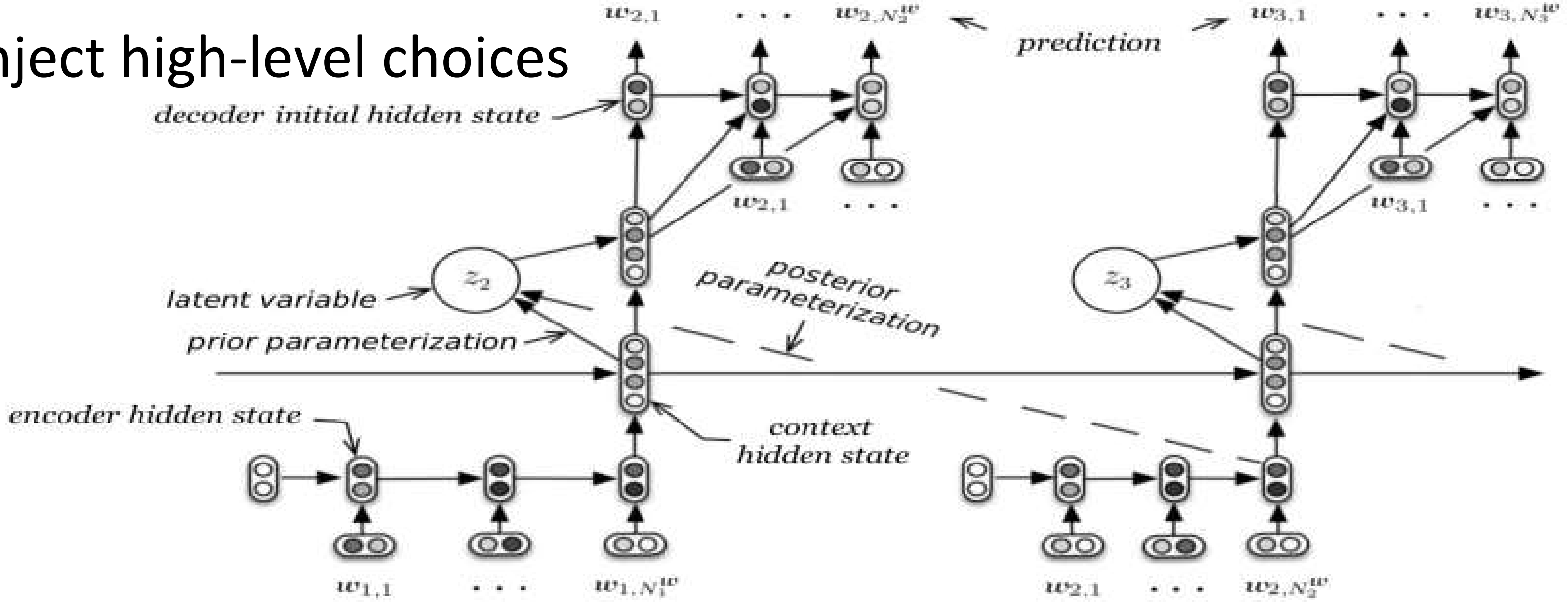
Table 3: Results on Gigaword Corpus for modeling UNK's with pointers in terms of recall.

	Rouge-1	Rouge-2	Rouge-L
NMT + lvt	36.45	17.41	33.90
NMT + lvt + PS	**37.29**	**17.75**	**34.70**

Text summarization

Variational Hierarchical RNNs for Dialogue Generation *(Serban et al 2016)*

- Lower level = words of an utterance (turn of speech)
- Upper level = state of the dialogue
- Inject high-level choices



Multi-Head Attention

We can run multiple attention mechanisms in parallel to focus on different aspects of the data

$$Attention(Q, K, V) = softmax\left(\frac{QK^T}{\sqrt{d_k}}\right)V$$

$$head_i = Attention(QW_i^Q, KW_i^K, VW_i^V).$$

$$MultiHeadAttention(Q, K, V) = Concat(head_1, \ldots, head_h)W^O$$

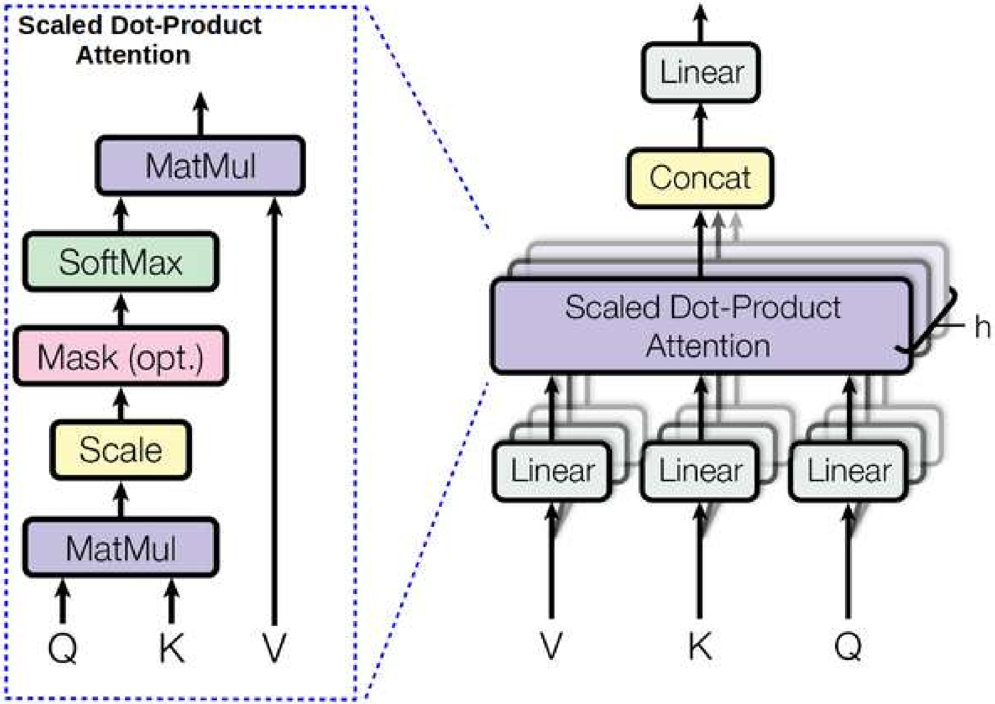


Fig: Michal Chromiak's blog

Self-Attention & Transformers

Vaswani et al Arxiv: 1706.03762

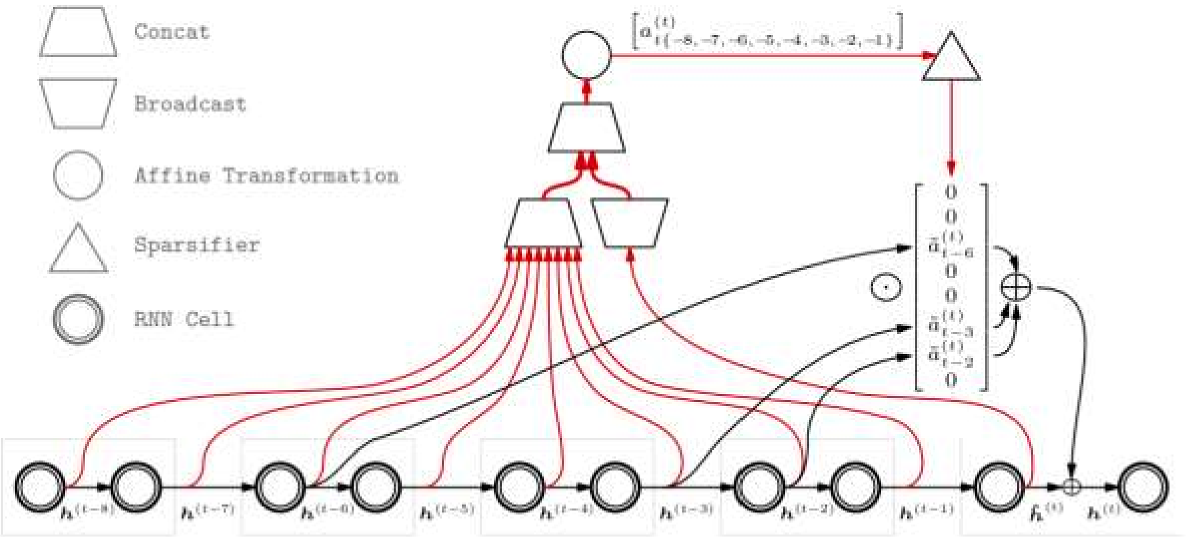
- **Parallelize** encoder
- Encode location of each item, no need for RNN
- Transform each location based on attention from all others
- See also Sparse Attentive Backtracking, Ke et al Arxiv:1711.02326

From: Jakob Uszkoreit, Google AI Blog, 2017

Using an Associative Memory to Bridge Large Time Spans and Avoid BPTT

Self-Attentive Backtracking, Ke et al Arxiv: 1711.02326

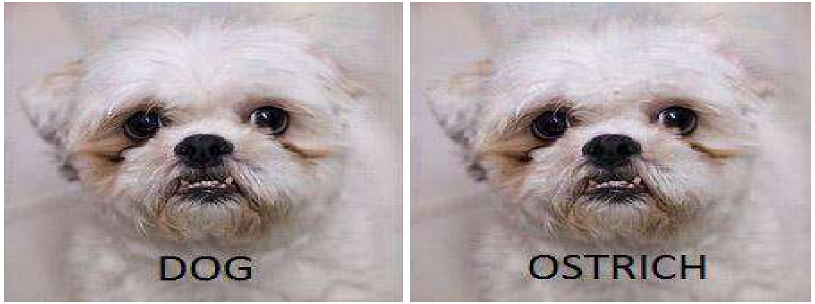
- Associate past and present events using a predictor, which acts like a trainable attentive skip connection between associated events
- Sparse attention to select few such events



May be a way for brains to avoid implausible BPTT

Still Far from Human-Level AI

- Industrial successes mostly based on **supervised** learning

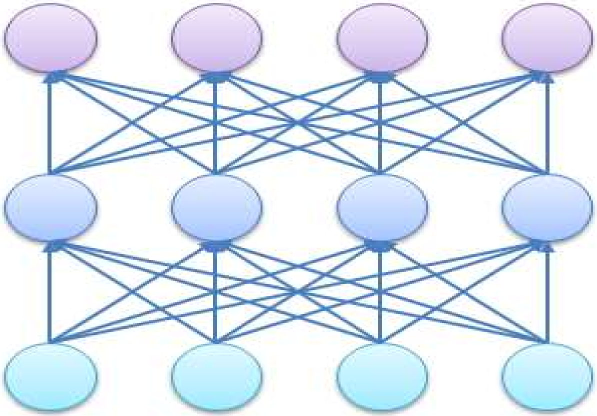


Adversarial example

- Learning superficial clues, not generalizing well outside of training contexts, easy to fool trained networks:
  - Current models cheat by picking on surface regularities
- Need to climb the ladder of higher-level abstractions

How to Discover Good Disentangled Representations

- How to discover abstractions?
- What is a good representation? ***(Bengio et al 2013)***
- Need clues (= priors) to help **disentangle** the underlying factors, e.g.
  - Spatial & temporal scales
  - Marginal independence
  - Simple dependencies between factors
    - *Consciousness prior*
  - Causal / mechanism independence
    - *Controllable factors*



Acting to Guide Representation Learning & Disentangling

(E. Bengio et al, 2017; V. Thomas et al, 2017)

- **Some factors (e.g. objects) correspond to 'independently controllable' aspects of the world**
- *Can only be discovered by acting in the world*
  - *Control linked to notion of objects & agents*
  - *Causal but agent-specific & subjective: affordances*

Abstraction Challenge for Unsupervised Learning

- Why is modeling P(acoustics) so much worse than modeling P(acoustics | phonemes) P(phonemes)?

- Wrong level of abstraction?
- **many more entropy bits in acoustic details then linguistic content**

→ predict the future in in abstract space instead: non-trivial

The Consciousness Prior

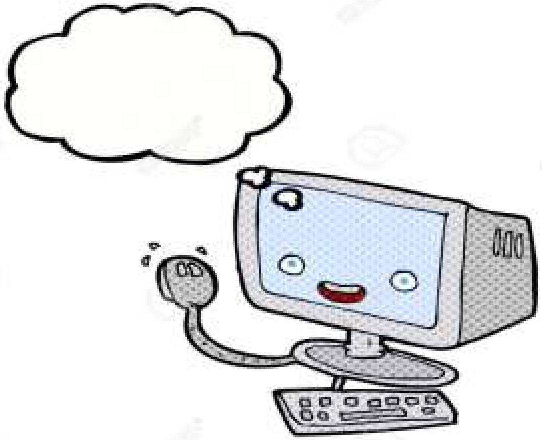
Bengio 2017, arXiv:1709.08568

- Conscious thoughts are very low-dimensional objects compared to the full state of the (unconscious) brain
- Yet they have unexpected predictive value or usefulness

  → strong constraint or prior on the und

- **Thought**: composition of few selected factors / concepts (key/value) at the highest level of abstraction of our brain

- Richer than but closely associated with short verbal expression such as a **sentence** or phrase, a **rule** or **fact** (link to classical symbolic AI & knowledge representation)



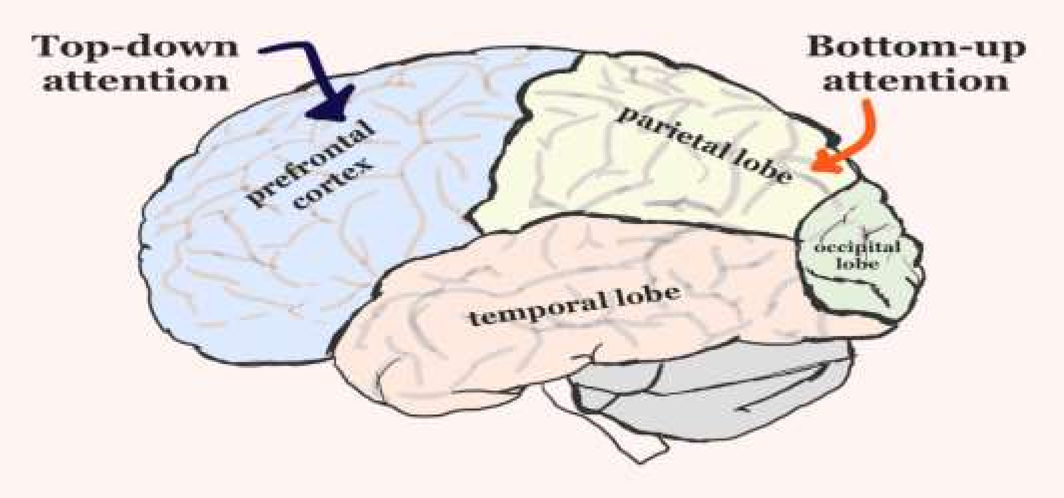
How to select a few relevant abstract concepts making a thought?

Content-based Attention

On the Relation between Abstraction and Attention

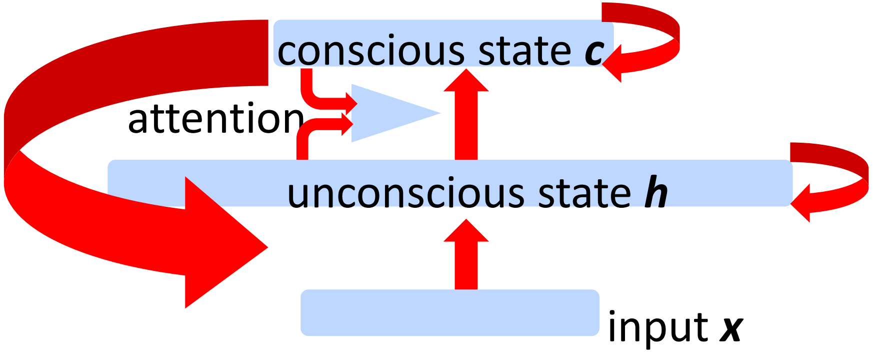
- Attention allows to focus on a few elements out of a large set
- Soft-attention allows this process to be trainable with gradient-based optimization and backprop

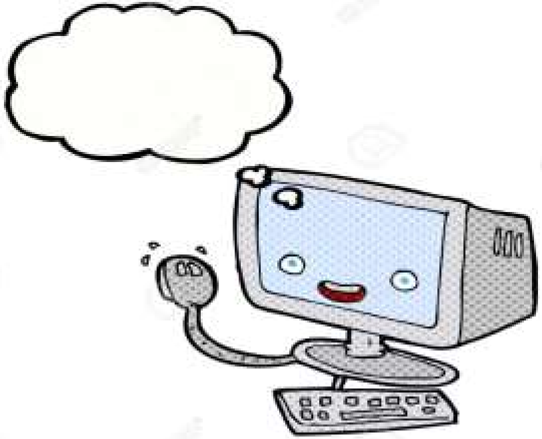
Attention focuses on a few appropriate abstract or concrete elements of mental representation



The Consciousness Prior
Bengio 2017, arXiv:1709.08568

- 2 levels of representation:
  - High-dimensional abstract representation space (all known concepts and factors) ***h***
  - Low-dimensional conscious thought ***c***,





Disentangling up to Linear Projection

- My old view of disentangling: each dimension of the representation = one 'nameable' (semantic) factor
- Potential problem: the number of 'nameable' factors is limited by the number of units, and brains don't use a completely localized representation for named things
- My current view of disentangling: it is enough that a linear projection exist to 'classify' or 'predict' any of the factors
- The 'number' of potential 'nameable' factors is now exponentially larger (e.g. subsets of dimensions, weights of these projections)

The Consciousness Prior

Bengio 2017, arXiv:1709.08568

- Conscious prediction over attended variables *A* (soft attention)

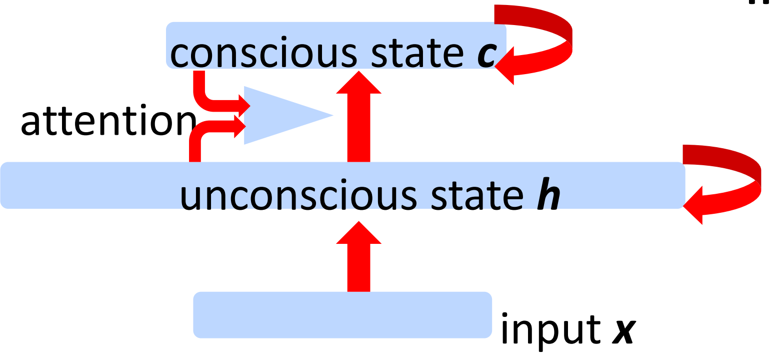
$$V = -\sum_A w_A \log P(h_{t,A} = a | c_{t-1})$$

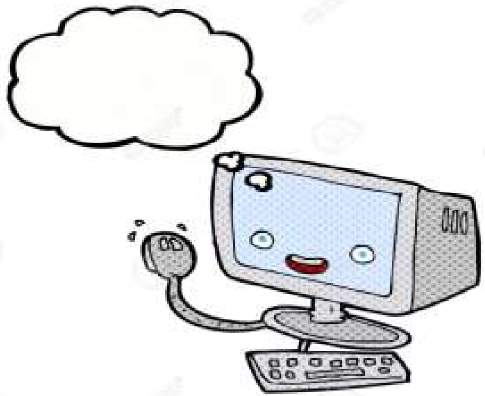
Attention weights

Factor **name**

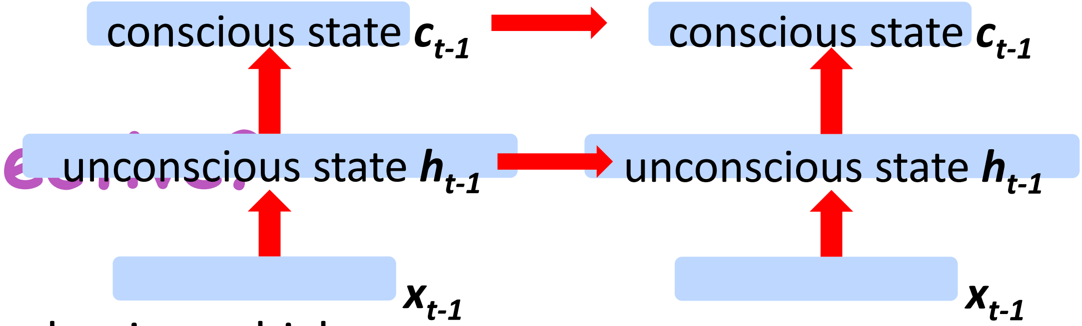
Predicted **value**

Earlier conscious state





What Training Objective?



- How to train the attention mechanism which selects which variables to predict?
  - Representation learning without reconstruction:
    - Maximize entropy of code
    - Maximize mutual information between past and future
  - *Objective function completely in abstract space, higher-level parameters model dependencies in abstract space*
  - *Usefulness of thoughts: as conditioning information for action, i.e., a particular form of planning for RL, i.e., the estimated gradient of rewards could also be used to drive learning of abstract representations*

Mila

Montreal Institute for Learning Algorithms

Université de Montréal