M2177.003100
Deep Learning

[10: Recurrent Neural Nets (Part 1)]

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(last compiled at 22:58:00 on 2020/10/25)

Outline

References

- *Deep Learning* by Goodfellow, Bengio and Courville ▸ Link
  - Chapter 10 Sequence Modeling: Recurrent and Recursive Nets
- online resources:
  - *Deep Learning Specialization (coursera)* ▸ Link
  - *Stanford CS231n: CNN for Visual Recognition* ▸ Link
  - *Dive into Deep Learning* ▸ Link

Outline

Recurrent neural networks (RNNs)

- a family of neural networks for processing sequential data
- comparison:

	CNN	RNN
specialized for	grid of values **X** (*e.g.* image)	sequence of values[1] $\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(\tau)}$
scale to	wide and tall images	long sequences[2]
can process	images of variable size	sequences of variable length

[1] RNNs usually operate on minibatches of sequences with a different sequence length τ for each member of the minibatch, but we omit minibatch indices to simplify notation

[2] much longer sequences than would be practical for networks without sequence-based specialization

Sequential data examples

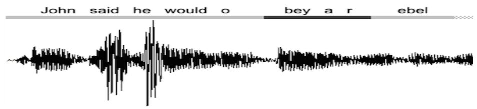
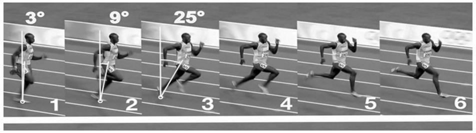
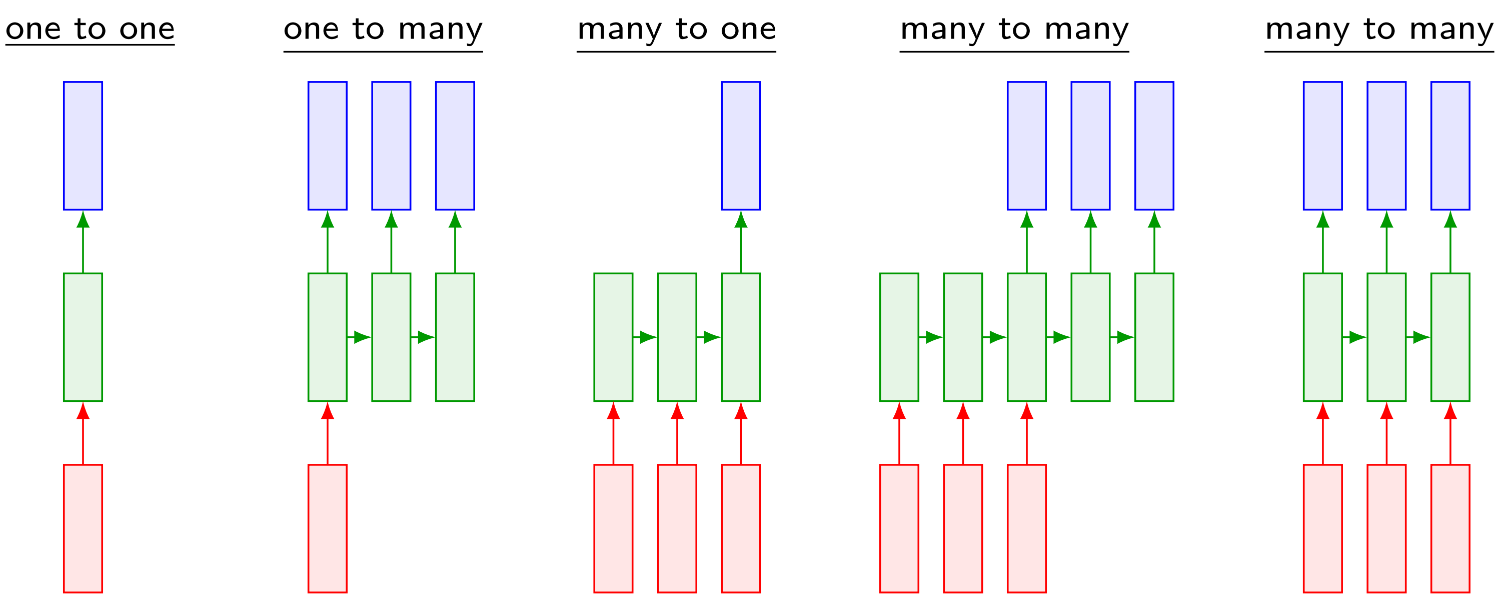
example	x	y
speech recognition		"John said he would obey a rebel."
music generation		
sentiment classification	"This movie is really, really fantastic."	★★★★★
DNA sequence	AAGTCTAACGTAAACGTCCCT	AAGTCTAACGTAAACGTCCCT
machine translation	¿Estás disfrutando de esta clase?	Are you enjoying this class?
video activity recognition		running
name entity recognition	Yesterday, Harry Potter met Hermione Granger.	Yesterday, Harry Potter met Hermione Granger.

image and table sources: doi.org/10.1044/2015_JSLHR-H-14-0239; images.app.goo.gl/wphsgrhALHZpjivZ7; images.app.goo.gl/iD6H8q8DcJCZgLocA; Ng, *Deep Learning* (Coursera), https://www.coursera.org/specializations/deep-learning

RNN modeling capability

e.g. **image captioning**
image $\rightarrow$ sentence

e.g. **machine translation**
seq of words $\rightarrow$ seq of words



vanilla neural net

e.g. **sentiment classification**
sentence $\rightarrow$ sentiment

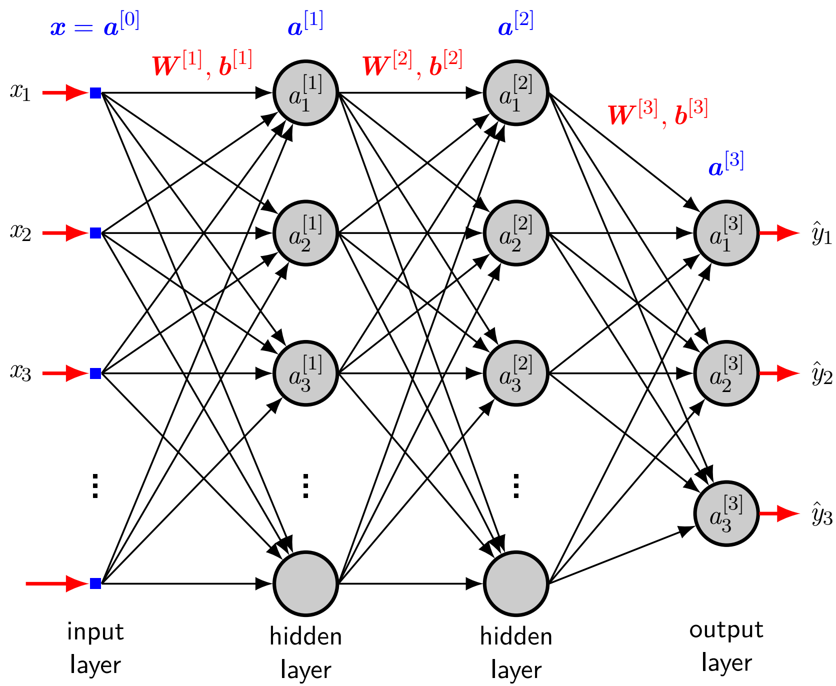
e.g. **video frame classification**
seq of frame $\rightarrow$ seq of class

image source: Fei-Fei Li, J. Johnson, S. Yeung, CS231n: Convolutional Neural Networks for Visual Recognition (2017), `http://cs231n.stanford.edu/2017/index.html`

Deep learning RNNaissance

image source: `https://www.youtube.com/watch?v=6bOMf9zr7N8`

Why not a vanilla neural net?



- problems
  - input/output: can be of different lengths
  - no sharing of features learned across different positions of sequence

image modified from: S. Haykin, *Neural Networks and Learning Machines*. Pearson Education, 3rd ed., 2010

Parameter sharing

- means: sharing parameters across different parts of a model
  - CNN: same kernel across image regions
  - RNN: same weights across time steps
- particularly important when
  - a specific piece of info can occur at multiple positions within the sequence
- benefits: the model can handle and generalize across
  - examples of different forms (*e.g.* different lengths in RNN)
- if we use separate parameters for each time index
  - cannot generalize to sequence lengths not seen during training
  - cannot share statistical strength across
    - different sequence lengths and different positions in time

Comparison

- 1D convolution over temporal sequences vs RNN:

	1D convolution	RNN
output	sequence	sequence
each member of output	a function of a small number of neighboring members of input	a function of the previous members of output
parameter sharing	same kernel at each time step	same update rule applied to outputs
depth	shallow	deep

Outline

Dynamical systems

- classical form of a dynamical system:

$$\boldsymbol{s}^{(t)} = f(\boldsymbol{s}^{(t-1)}; \boldsymbol{\theta}) \quad (1)$$

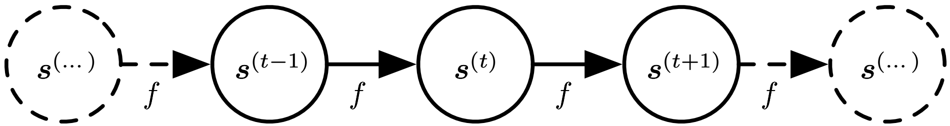
$$= f_{\boldsymbol{\theta}}(\boldsymbol{s}^{(t-1)}) \quad \text{(simplified notation)}$$

  - $\boldsymbol{s}^{(t)}$: state of the system
  - function f maps state at $t-1$ to state at t (parameterized by $\boldsymbol{\theta}$)
  - "recurrent"
    - definition of s at time t refers back to same definition at time $t-1$

- unfolding (1) for $\tau = 3$ time steps gives

$$s^{(3)} = f_{\theta}(s^{(2)}) = f_{\theta}(f_{\theta}(s^{(1)}))$$

  - does not involve recurrence
  - can be represented by a directed acyclic computational graph



  - note: same parameter θ used for all time steps

- another example: consider a dynamical system

$$s^{(t)} = f_{\theta}(s^{(t-1)}, x^{(t)}) \tag{2}$$

  - driven by external signal $x^{(t)}$

$\Rightarrow$ state now contains information about the whole past sequence

image source: I. Goodfellow, Y. Bengio, and A. Courville, *Deep learning*. MIT Press, 2016

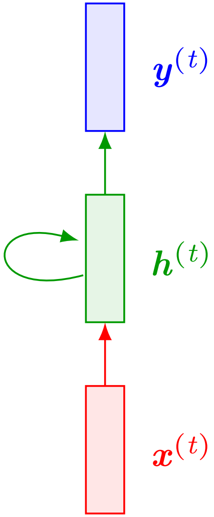
Outline

Recurrent neural net (RNN)

- rewrite (2) using variable $\boldsymbol{h}$ to represent the state:

$$\underbrace{\boldsymbol{h}^{(t)}}_{\text{new state}} = f_{\boldsymbol{\theta}}(\underbrace{\boldsymbol{h}^{(t-1)}}_{\text{old state}}, \underbrace{\boldsymbol{x}^{(t)}}_{\text{input}})$$

  - the state consists of hidden units
  - same f, same $\boldsymbol{\theta}$ at every time step



- typical RNNs add extra architectural features

  e.g. output layers: read info out of $\boldsymbol{h}$ to make predictions

$$\boldsymbol{y}^{(t)} = \sigma(\boldsymbol{W}\boldsymbol{h}^{(t)})$$

- what is the role of hidden units?

image source: Fei-Fei Li, J. Johnson, S. Yeung, CS231n: Convolutional Neural Networks for Visual Recognition (2017), http://cs231n.stanford.edu/2017/index.html

Hidden states as a lossy summary

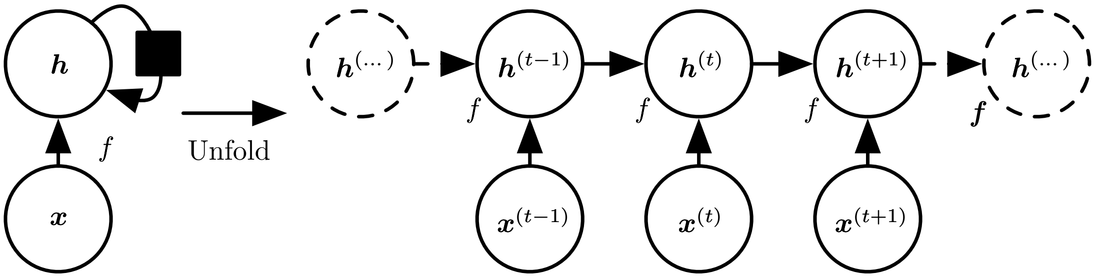
- assume a task: predicting future from past using an RNN
- the net learns to use $\boldsymbol{h}^{(t)}$ as a "lossy summary"
  - of task-relevant aspects of the past sequence of inputs up to t
- this summary
  - maps $\underbrace{\boldsymbol{x}^{(t)}, \boldsymbol{x}^{(t-1)}, \ldots, \boldsymbol{x}^{(2)}, \boldsymbol{x}^{(1)}}_{\text{arbitrary length sequence}}$ to $\underbrace{\boldsymbol{h}^{(t)}}_{\text{fixed length vector}}$ $\Rightarrow$ necessarily lossy
  - may selectively keep some aspects of past sequence (more precisely)

e.g. language modeling (predicting next word given previous words)

$\rightarrow$ store only enough info for prediction (not entire input sentence)

- most demanding situation (*e.g.* autoencoders in ch 14)
  - $\boldsymbol{h}^{(t)}$ should be rich enough to approximately recover the input sequence

Two ways to draw an RNN



1. recurrent graph (circuit diagram): left
   - black square: a delay of a single time step
2. unfolded graph: right
   - each node: now associated with one particular time instance

- this RNN just processes information from input x by
  - incorporating it into state h that is passed forward through time

image source: I. Goodfellow, Y. Bengio, and A. Courville, *Deep learning*. MIT Press, 2016

- we can represent unfolded recurrence after t steps with a function $g^{(t)}$:

$$
\begin{aligned}
\boldsymbol{h}^{(t)} &= g^{(t)}(\overbrace{\boldsymbol{x}^{(t)}, \boldsymbol{x}^{(t-1)}, \boldsymbol{x}^{(t-2)}, \ldots, \boldsymbol{x}^{(2)}, \boldsymbol{x}^{(1)}}^{\text{the whole past sequence as input}}) \\
&= f_{\boldsymbol{\theta}}(\boldsymbol{h}^{(t-1)}, \boldsymbol{x}^{(t)})
\end{aligned}
$$

- we learn f rather than $g^{(t)}$
  - f: a single model that operates on all time steps/all sequence lengths
    - same input size regardless of sequence length[3]
  - $g^{(t)}$: a separate model for all possible time steps

- advantages of learning the same transition function f
  - generalization (to sequence lengths not seen in training)
  - requires far fewer training examples (thanks to parameter sharing)

[3] f is specified in terms of transition from one state to another rather than a variable-length history of states

Simple/vanilla/Elman RNN

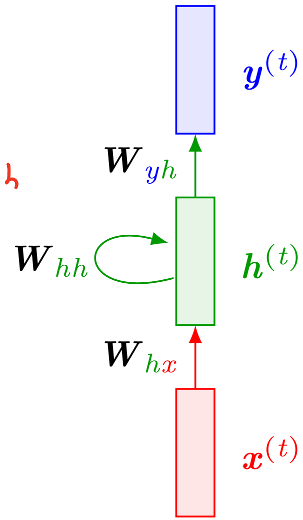
f : tanh

θ : W_{hh}, W_{hx}, b_h, W_{yh}, b_y

$$\underbrace{\boldsymbol{h}^{(t)}}_{\text{new state}} = f_{\boldsymbol{\theta}}(\underbrace{\boldsymbol{h}^{(t-1)}}_{\text{old state}}, \underbrace{\boldsymbol{x}^{(t)}}_{\text{input}})$$

$$= \tanh(\boldsymbol{W}_{hh}\boldsymbol{h}^{(t-1)} + \boldsymbol{W}_{hx}\boldsymbol{x}^{(t)} + \boldsymbol{b}_h)$$

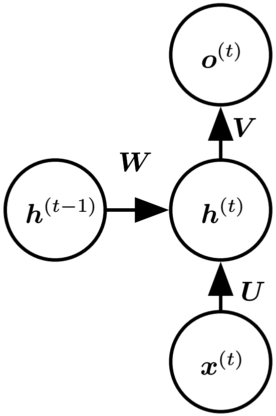
$$\boldsymbol{y}^{(t)} = \mathrm{softmax}(\boldsymbol{W}_{yh}\boldsymbol{h}^{(t)} + \boldsymbol{b}_y)$$



- system state
  - consists of a single hidden vector $\boldsymbol{h}^{(t)}$
- parameter sharing
  - <u>Same</u> parameters $(\underbrace{\boldsymbol{W}_{hx}, \boldsymbol{W}_{hh}, \boldsymbol{W}_{yh},}_{\text{weight matrices}} \underbrace{\boldsymbol{b}_h, \boldsymbol{b}_y}_{\text{bias vectors}})$ at every time step
- activation: may vary from architecture to architecture

image source: Fei-Fei Li, J. Johnson, S. Yeung, CS231n: Convolutional Neural Networks for Visual Recognition (2017), http://cs231n.stanford.edu/2017/index.html

Alternative notation (textbook)



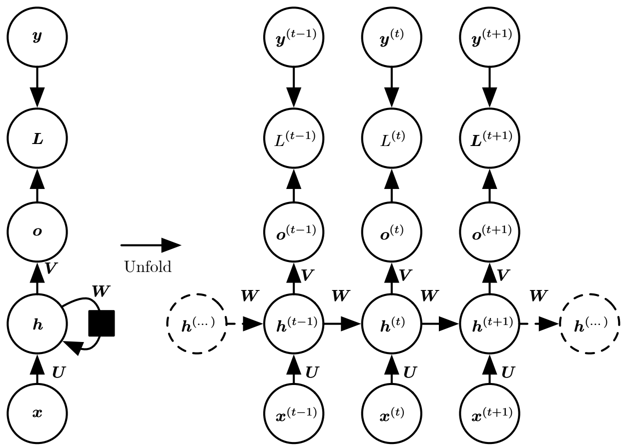
$$\boldsymbol{a}^{(t)} = \boldsymbol{b} + \boldsymbol{W}\boldsymbol{h}^{(t-1)} + \boldsymbol{U}\boldsymbol{x}^{(t)}$$
$$\boldsymbol{h}^{(t)} = \tanh(\boldsymbol{a}^{(t)})$$
$$\boldsymbol{o}^{(t)} = \boldsymbol{c} + \boldsymbol{V}\boldsymbol{h}^{(t)}$$
$$\hat{\boldsymbol{y}}^{(t)} = \mathrm{softmax}(\boldsymbol{o}^{(t)})$$

- $\boldsymbol{b}, \boldsymbol{c}$: bias vectors
- $\underbrace{\boldsymbol{U}}_{\text{input-to-hidden}}, \underbrace{\boldsymbol{V}}_{\text{hidden-to-output}}, \underbrace{\boldsymbol{W}}_{\text{hidden-to-hidden}}$: weight matrices

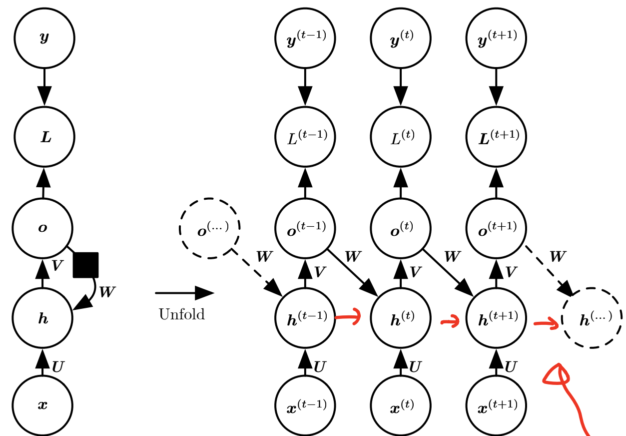
image source: I. Goodfellow, Y. Bengio, and A. Courville, *Deep learning*. MIT Press, 2016

Two types of recurrence structures

- hidden-to-hidden



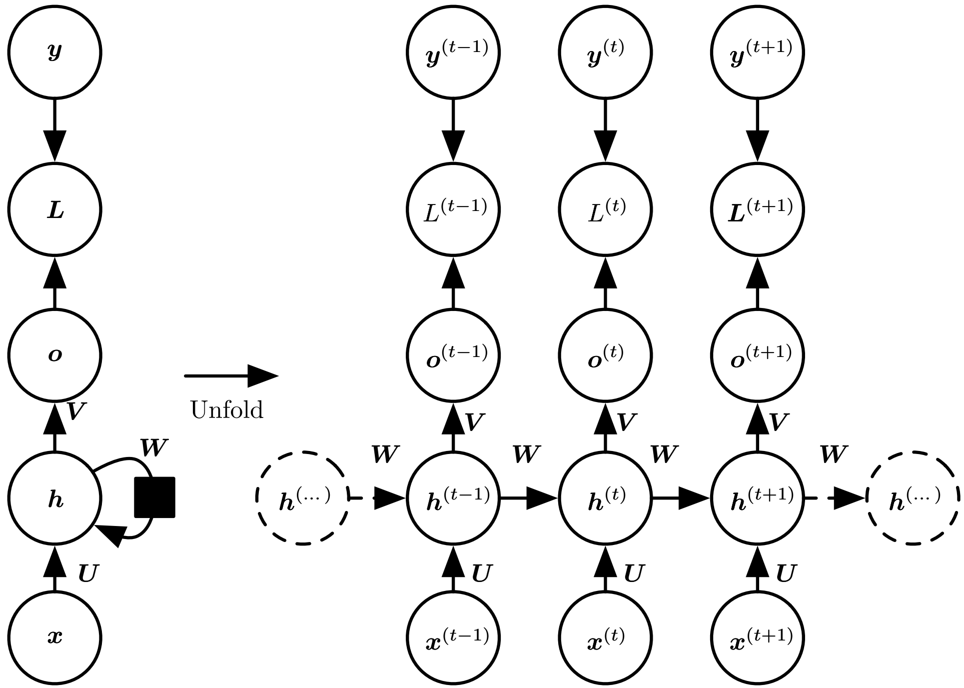
- output-to-hidden



▶ it is possible to have both types simultaneously

image source: I. Goodfellow, Y. Bengio, and A. Courville, *Deep learning*. MIT Press, 2016

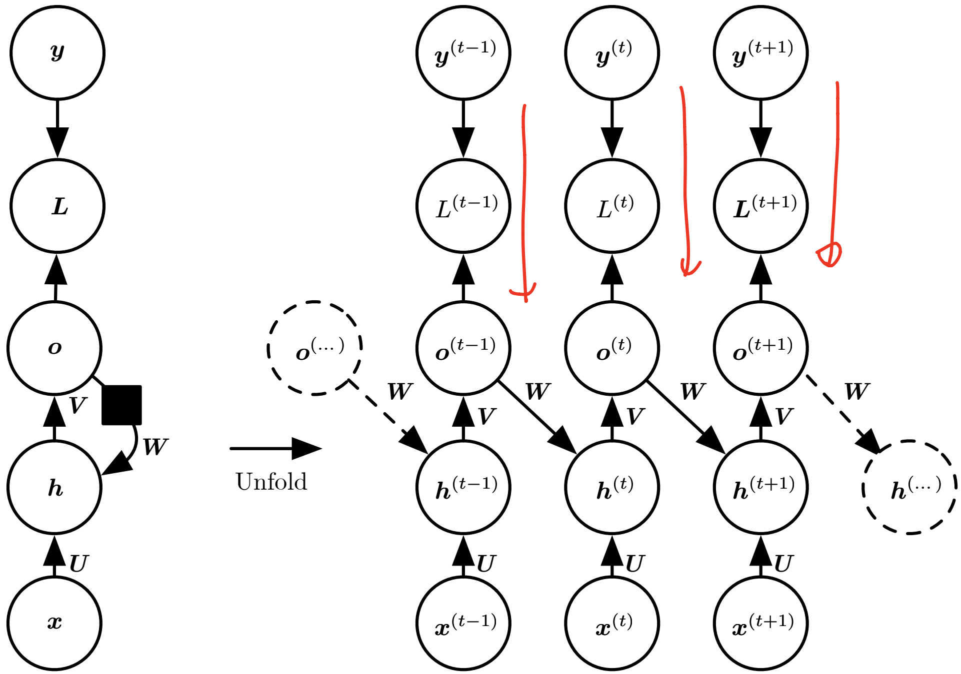
hidden-to-hidden recurrence



- most popular, representative architecture
  - a universal RNN that simulates a Turing machine (see textbook)

image source: I. Goodfellow, Y. Bengio, and A. Courville, *Deep learning*. MIT Press, 2016

output-to-hidden recurrence



- less expressive than the previous type (unless $\boldsymbol{o}$ is very high-dim and rich)
  - but training is easier (each time step trained independently in parallel)

image source: I. Goodfellow, Y. Bengio, and A. Courville, *Deep learning*. MIT Press, 2016

Outline

RNN training

- three types
  - teacher forcing
  - backprop through time (BPTT)
  - real-time recurrent learning (RTRL)
- teacher forcing[4]
  - for nets with output-hidden but without hidden-hidden connections
  - motivated by computational burden of BPTT
- BPTT: most widely used (can train hidden-to-hidden architecture)
  - essentially truncated backprop on unfolded graph
- RTRL: training while forward prop
  - no backprop needed but computationally expensive (not used in practice)

[4] c.f. knowledge distillation (see page 36)

Forward propagation

- assume a vanilla RNN
  - for $t = 0$: specify initial state $\boldsymbol{h}^{(0)}$
  - for each time step (from $t = 1$ to $t = \tau$): apply updates

$$\boldsymbol{h}^{(t)} = \tanh(\boldsymbol{W}_{hh}\boldsymbol{h}^{(t-1)} + \boldsymbol{W}_{hx}\boldsymbol{x}^{(t)} + \boldsymbol{b}_h)$$

$$\hat{\boldsymbol{y}}^{(t)} = \text{softmax}(\boldsymbol{W}_{yh}\boldsymbol{h}^{(t)} + \boldsymbol{b}_y)$$

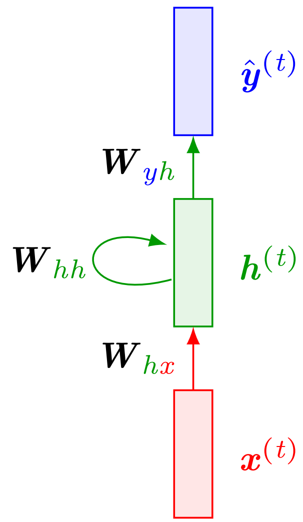
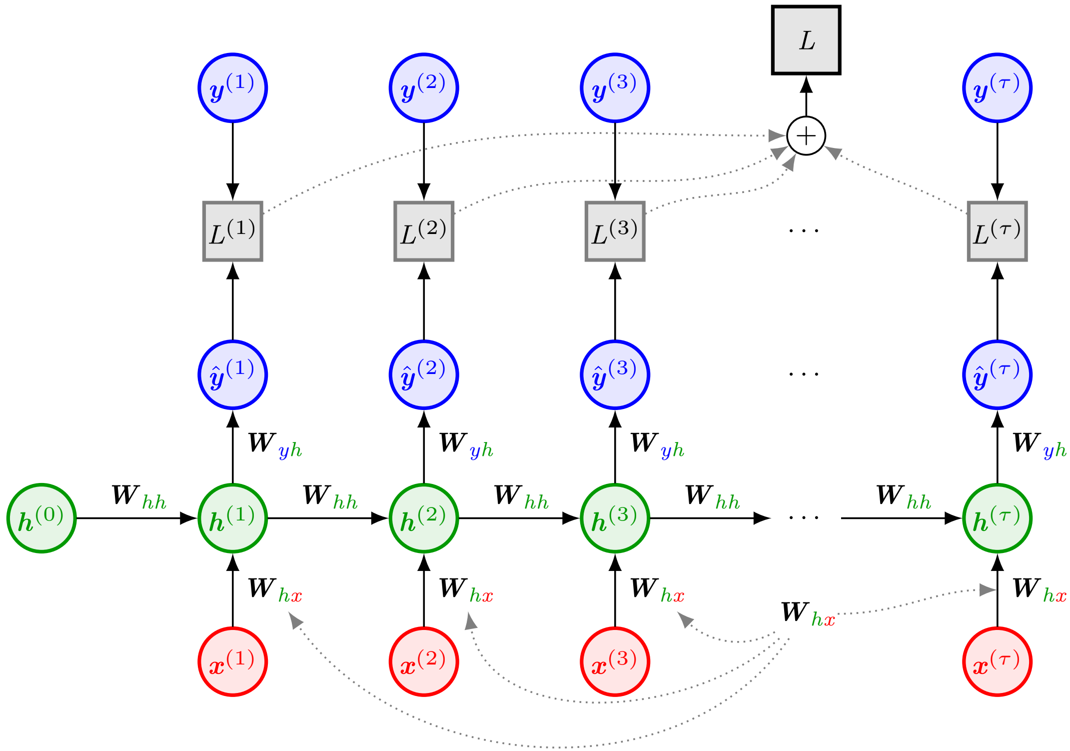


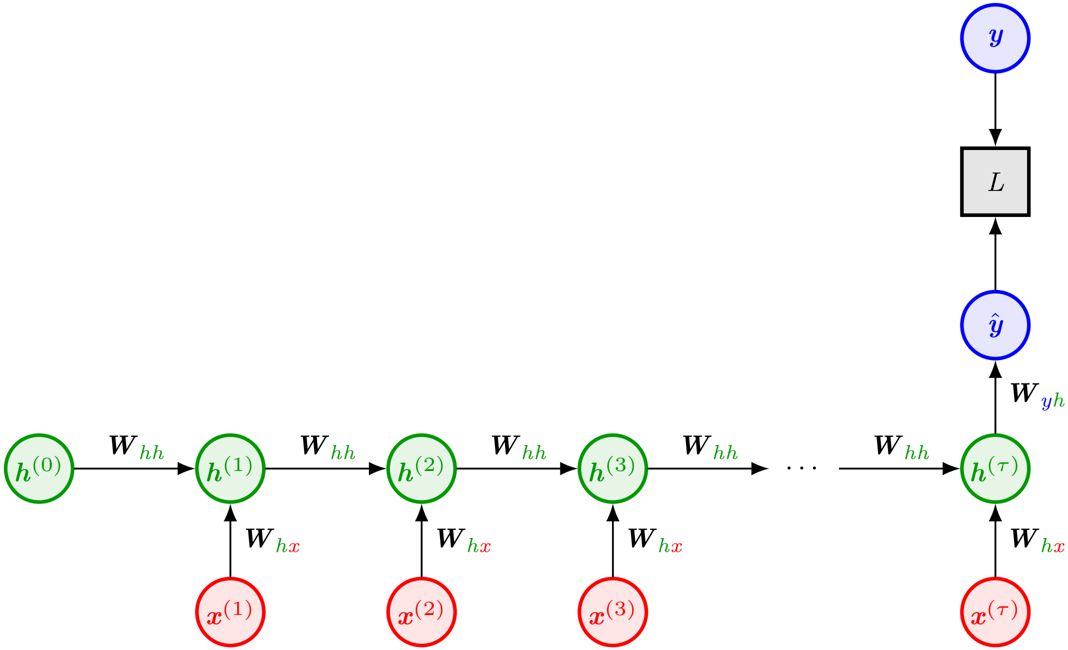
image source: Fei-Fei Li, J. Johnson, S. Yeung, CS231n: Convolutional Neural Networks for Visual Recognition (2017), http://cs231n.stanford.edu/2017/index.html

many-to-many



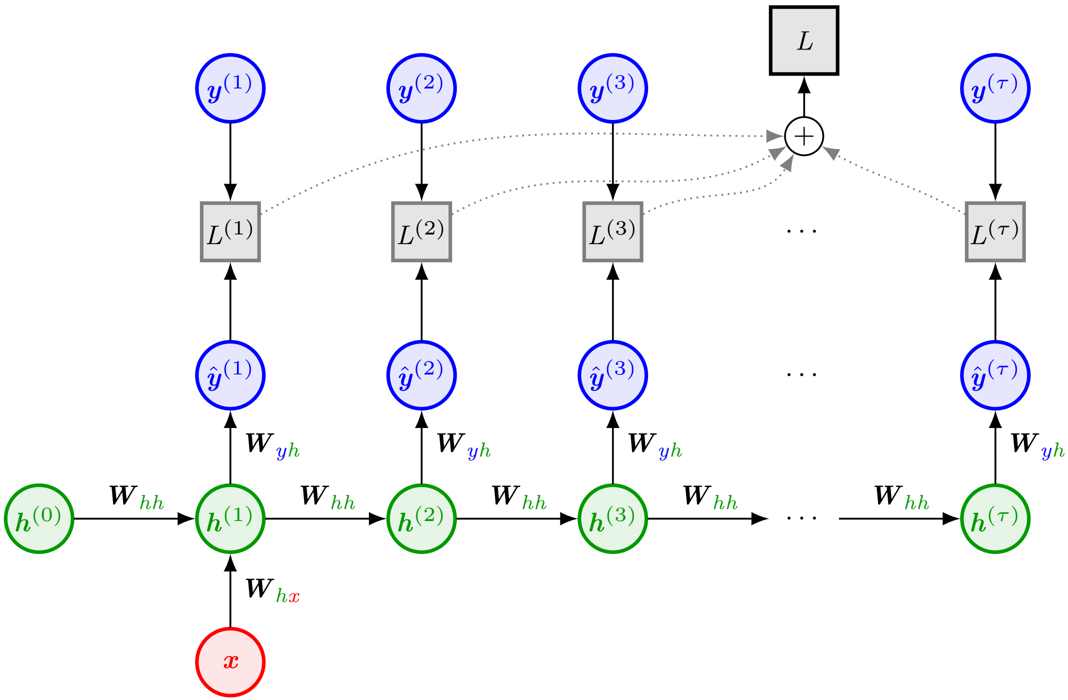
- total loss for a sequence of $\boldsymbol{x}$ (paired with same-length sequence $\boldsymbol{y}$)
  - sum of losses over all time steps: $L = \sum_{t=1}^{\tau} L^{(t)} = \sum_{t=1}^{\tau} L(\hat{\boldsymbol{y}}^{(t)}, \boldsymbol{y}^{(t)})$

many-to-one



- loss for a sequence of $\boldsymbol{x}$ (label: a single vector $\boldsymbol{y}$)
  - $L = L(\hat{\boldsymbol{y}}, \boldsymbol{y})$

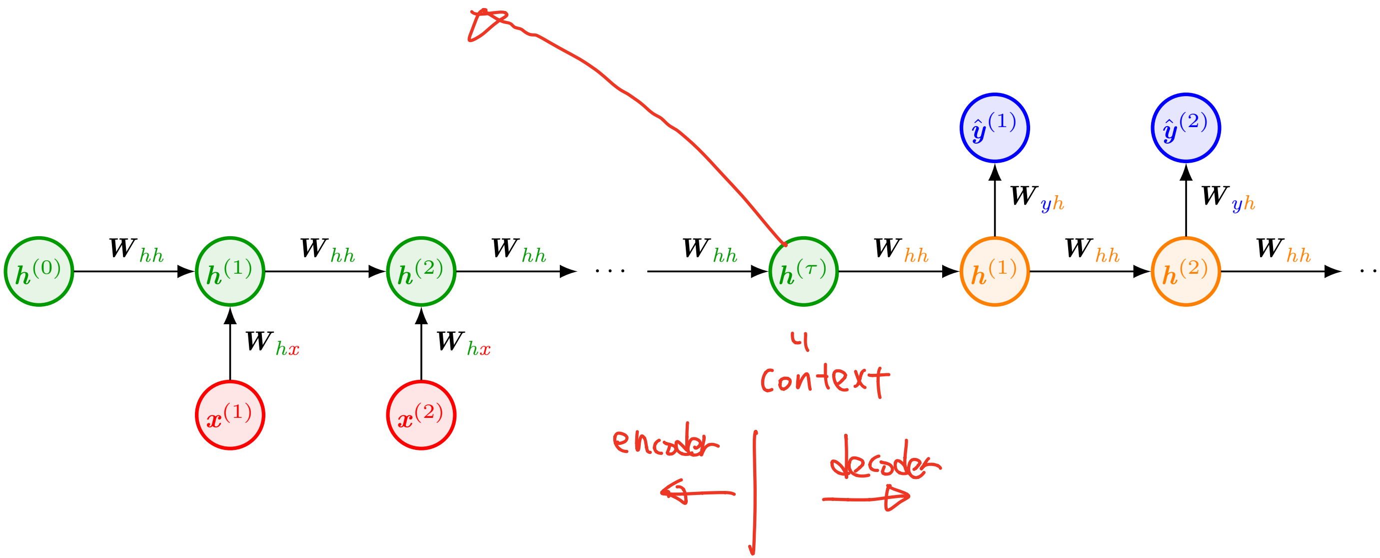
one-to-many



- total loss for a vector $\boldsymbol{x}$ (label: a sequence of $\boldsymbol{y}$)
  - sum of losses over all time steps: $L(\hat{\boldsymbol{y}}, \boldsymbol{y}) = \sum_{t=1}^{\tau} L^{(t)} = \sum_{t=1}^{\tau} L(\hat{\boldsymbol{y}}^{(t)}, \boldsymbol{y}^{(t)})$

$\boxed{\text{sequence-to-sequence}}$ (= many-to-one + one-to-many)

- many-to-one
  - encode input sequence into a single vector
- one-to-many
  - produce output sequence from the single input vector



- two RNNs: trained jointly (more on this later)

BPTT: computing gradient through RNN

- use of backprop on unrolled graph: called BPTT (backprop through time)
  - forward prop through entire sequence → compute loss
  - backprop through entire sequence → compute $\underbrace{\text{gradient}}$

↑

may then be used with any general-purpose gradient-based techniques to train an RNN

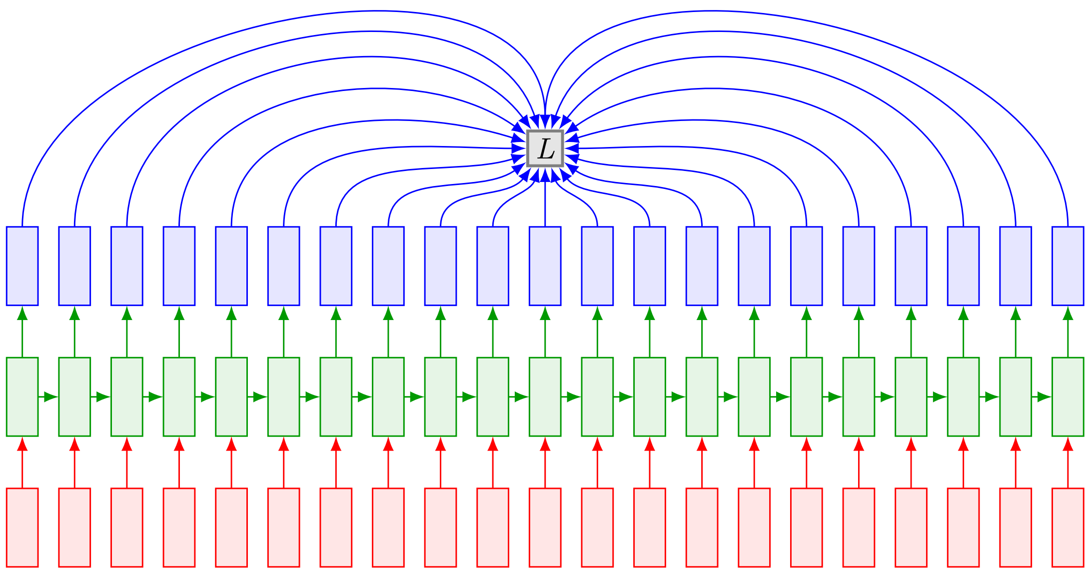


image modified from: Fei-Fei Li, J. Johnson, S. Yeung, CS231n: Convolutional Neural Networks for Visual Recognition (2017), http://cs231n.stanford.edu/2017/index.html

Computational cost

- computing $\nabla_{\boldsymbol{\theta}} L$
  - an expensive operation
  - involves both forward/backward propagation through graph
- runtime: $O(\tau)$ and cannot be reduced by parallelization
  - forward prop graph: inherently sequential

  i.e. each time step may only be computed after the previous one
- memory: also $O(\tau)$
  - states computed in fwd pass must be stored until reused during bwd pass
- the network with recurrence between hidden units:
  - thus very powerful but also expensive to train

Truncated BPTT

- run forward/backward through chunks of sequence (instead of whole sequence)
  - carry hidden states forward in time forever
  - but only backpropagate for some smaller number of steps
  - in spirit: similar to minibatch sgd

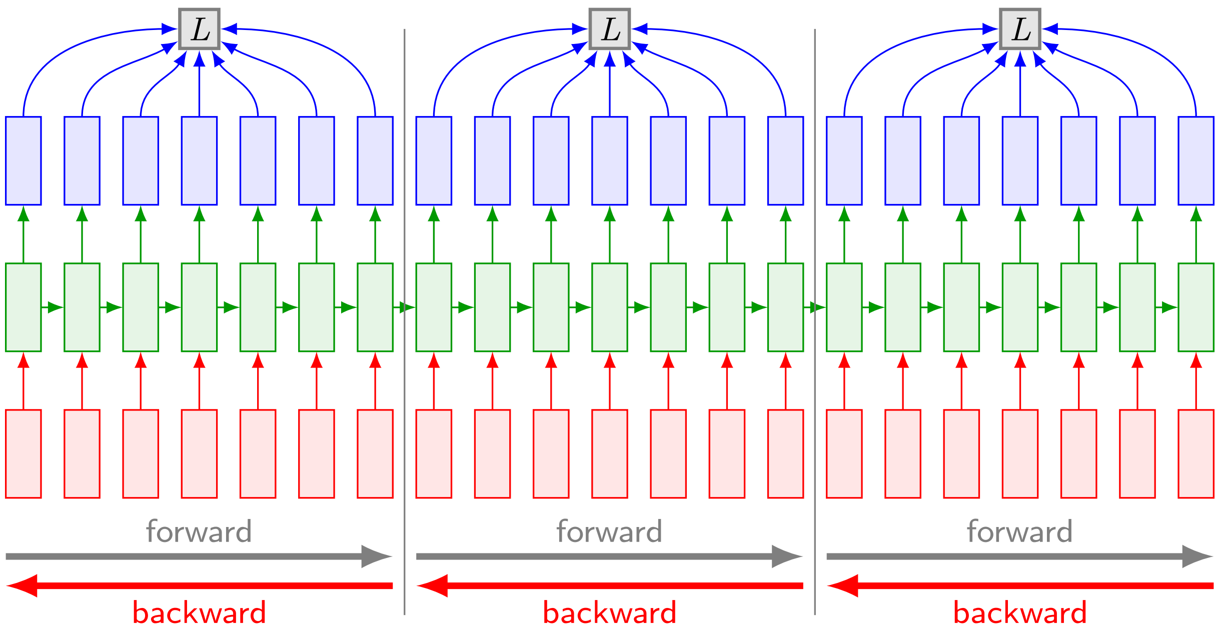
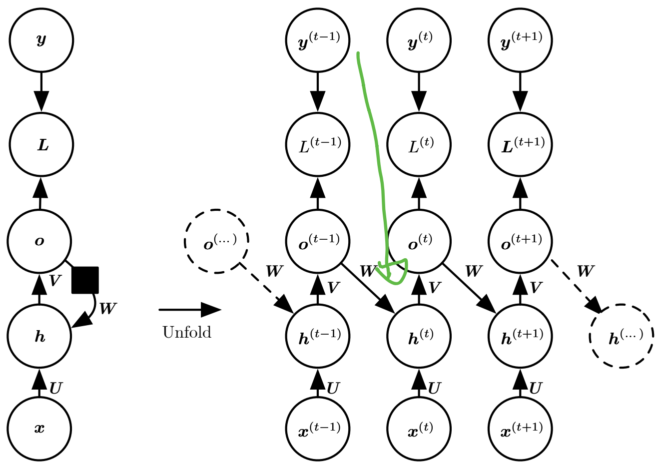


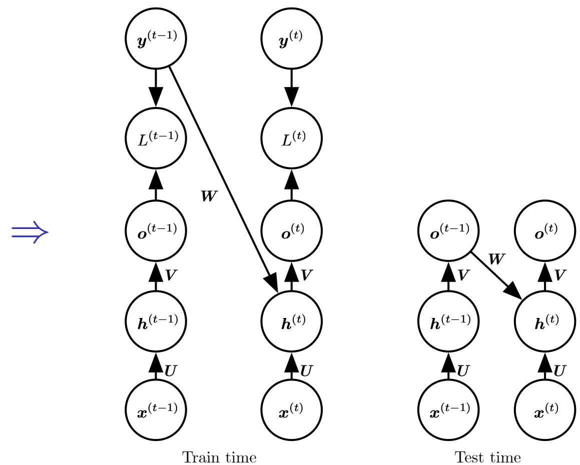
image modified from: Fei-Fei Li, J. Johnson, S. Yeung, CS231n: Convolutional Neural Networks for Visual Recognition (2017), http://cs231n.stanford.edu/2017/index.html

Teacher forcing

- a training technique for nets with output-hidden recurrence
  - ▸ no hidden-to-hidden recurrence (→ less expressive)
  - ▸ each time step can be trained independently in parallel (→ faster)
- what it does
  - ▸ training: ground truth output $\boldsymbol{y}^{(t-1)}$ as input at time t
  - ▸ testing: model output $\hat{\boldsymbol{y}}^{(t-1)}$ as input at time t



RNN to train



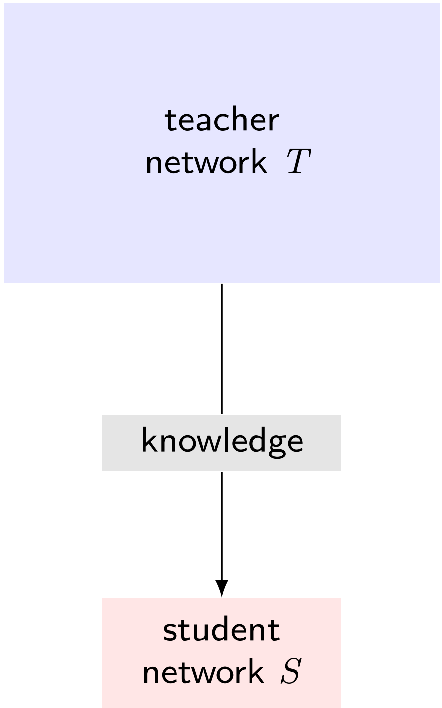
teacher forcing

image source: I. Goodfellow, Y. Bengio, and A. Courville, *Deep learning*. MIT Press, 2016

Digression: knowledge distillation

- proposed context: model deployment
- teacher net (T): "cumbersome" model

  e.g. a large ensemble
  - (pros) excellent performance
  - (cons) computationally expensive
  - cannot be deployed in limited environments
- student net (S): "small" model
  - suitable for deployment
  - (pros) fast inference
  - (cons) lower performance than T
- knowledge: soft label ("**dark knowledge**") of T



source: Geoffrey Hinton, Oriol Vinyals, and Jeff Dean. "Distilling the knowledge in a neural network". In: *arXiv preprint arXiv:1503.02531* (2015) https://arxiv.org/abs/1503.02531

Outline

Language modeling

- central to many important natural language processing (NLP)
  - ▸ used to generate text in various NLP tasks

  e.g. speech recognition, machine translation, image captioning, spelling correction, text summarization, ...

- major tasks (← inherently probabilistic)
  - ▸ assign probability to sentences in a language

$$P(\text{apple and pair salad}) = 3.2 \times 10^{-13}$$
$$P(\text{apple and pear salad}) = 5.7 \times 10^{-10}$$

  - ▸ predict the next word in a sequence given the words that precede it

$$P(\text{pair} \mid \text{apple and}) = 0.00012$$
$$P(\text{pear} \mid \text{apple and}) = 0.03$$

- major types
  - (classical) statistical language model (*e.g.* n-gram)
  - neural language model (NLM) (*e.g.* word embedding)

- key reason for improved performance by NLM
  - ability to generalize

- NLM learns directly from raw text data
  - both $\underbrace{\text{representation}}_{\substack{\uparrow \\ \text{word feature vector}}}$ and $\underbrace{\text{probabilistic model}}_{\substack{\uparrow \\ \text{language model + its parameters}}}$

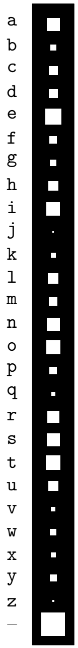
- NLM addresses the n-gram data sparsity issue through
  - parameterizing words as vectors (*i.e.* word embedding)
  - using them as inputs to a neural net

Character-level n-gram examples

- corpus: *The frequently Asked Questions Manual for Linux*

- monogram
  - $p(x)$

i	a_i	p_i
1	a	0.0575
2	b	0.0128
3	c	0.0263
4	d	0.0285
5	e	0.0913
6	f	0.0173
7	g	0.0133
8	h	0.0313
9	i	0.0599
10	j	0.0006
11	k	0.0084
12	l	0.0335
13	m	0.0235
14	n	0.0596
15	o	0.0689
16	p	0.0192
17	q	0.0008
18	r	0.0508
19	s	0.0567
20	t	0.0706
21	u	0.0334
22	v	0.0069
23	w	0.0119
24	x	0.0073
25	y	0.0164
26	z	0.0007
27	–	0.1928



- bigram
  - $p(xy)$

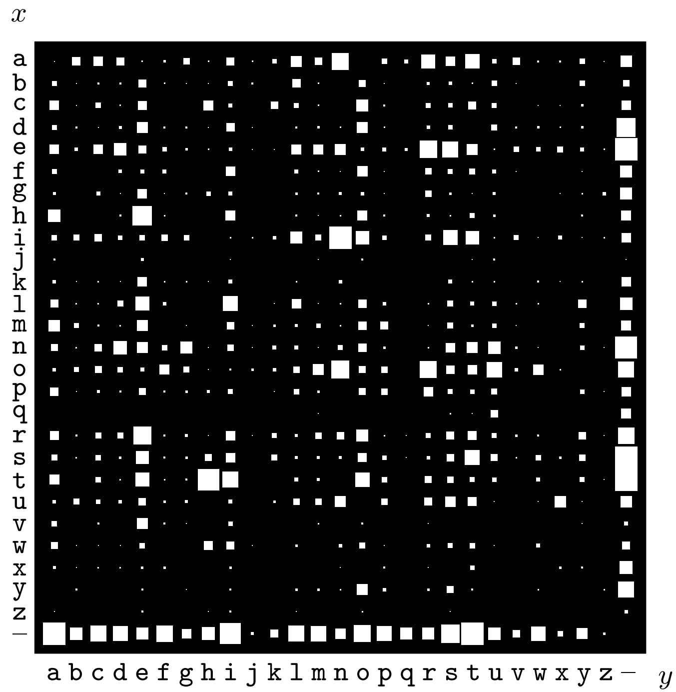
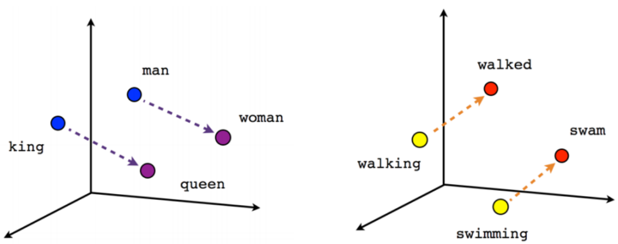
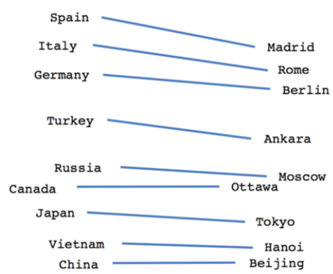


image source: David JC MacKay. *Information theory, inference and learning algorithms*. Cambridge university press, 2003

Word embedding (word2vec, GloVe, ELMo)

- learned representation of words based on usage
  - uses a real-valued vector to represent each word (dense vector)
  - allows words with a similar meaning to have a similar representation





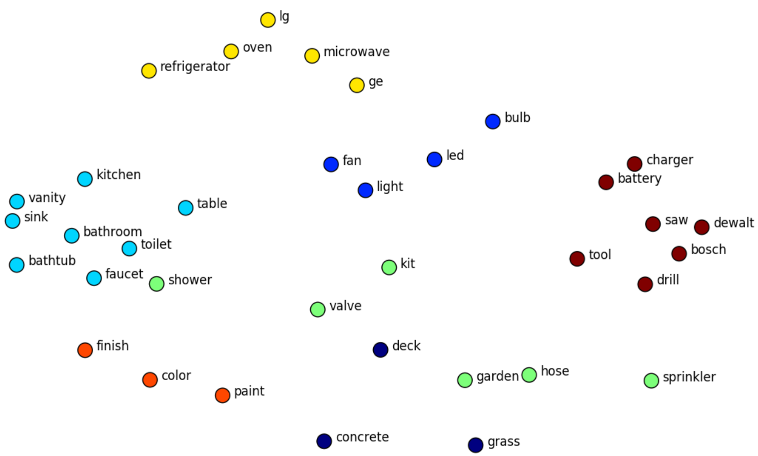


image sources: https://images.app.goo.gl/T2M4c3jMMY39p26a6; https://images.app.goo.gl/cBTLHGzFDe7FLxBH7

RNN-based language modeling

- training data: text **corpus** (a large and structured set of texts)

step 1: tokenization

- input sentence $\mapsto$ individual tokens in your vocabulary

e.g. `The pen is mightier than the sword.`

The	pen	is	mightier	than	the	sword	.	<EOS>
$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$
$\boldsymbol{y}^{(1)}$	$\boldsymbol{y}^{(2)}$	$\boldsymbol{y}^{(3)}$	$\boldsymbol{y}^{(4)}$	$\boldsymbol{y}^{(5)}$	$\boldsymbol{y}^{(6)}$	$\boldsymbol{y}^{(7)}$	$\boldsymbol{y}^{(8)}$	$\boldsymbol{y}^{(9)}$

- special cases
  - start of sentence: `<SOS>`
  - end of sentence: `<EOS>`
  - unknown word: `<UNK>`

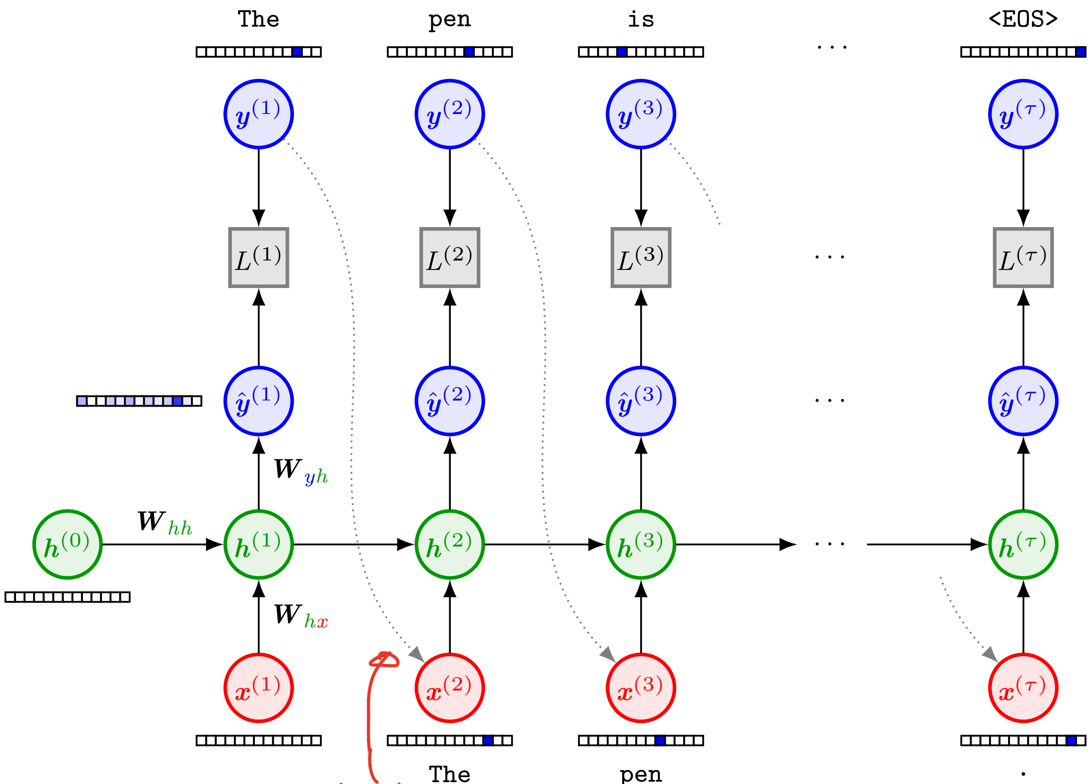
step 2: supervised training

- use RNN to model the probability of different token sequences
- architecture
  - real output $\boldsymbol{y}^{(t)}$: vocabulary-size one-hot vector
  - model output $\hat{\boldsymbol{y}}^{(t)}$: vocabulary-size softmax vector
  - if we use a vanilla RNN

$$
\begin{aligned}
\boldsymbol{x}^{(t)} &= \boldsymbol{y}^{(t-1)} \\
\boldsymbol{h}^{(t)} &= \tanh(\boldsymbol{W}_{hh}\boldsymbol{h}^{(t-1)} + \boldsymbol{W}_{hx}\boldsymbol{x}^{(t)} + \boldsymbol{b}_h) \\
&= \tanh(\boldsymbol{W}_{hh}\boldsymbol{h}^{(t-1)} + \boldsymbol{W}_{hx}\boldsymbol{y}^{(t-1)} + \boldsymbol{b}_h) \\
\hat{\boldsymbol{y}}^{(t)} &= \mathrm{softmax}(\boldsymbol{W}_{yh}\boldsymbol{h}^{(t)} + \boldsymbol{b}_y)
\end{aligned}
$$

  - initialization: $\boldsymbol{x}^{(1)} = \mathbf{0}$, $\boldsymbol{h}^{(0)} = \mathbf{0}$
  - loss: *e.g.* cross-entropy loss (see next page)

- example: `The pen is mightier than the sword.<EOS>`



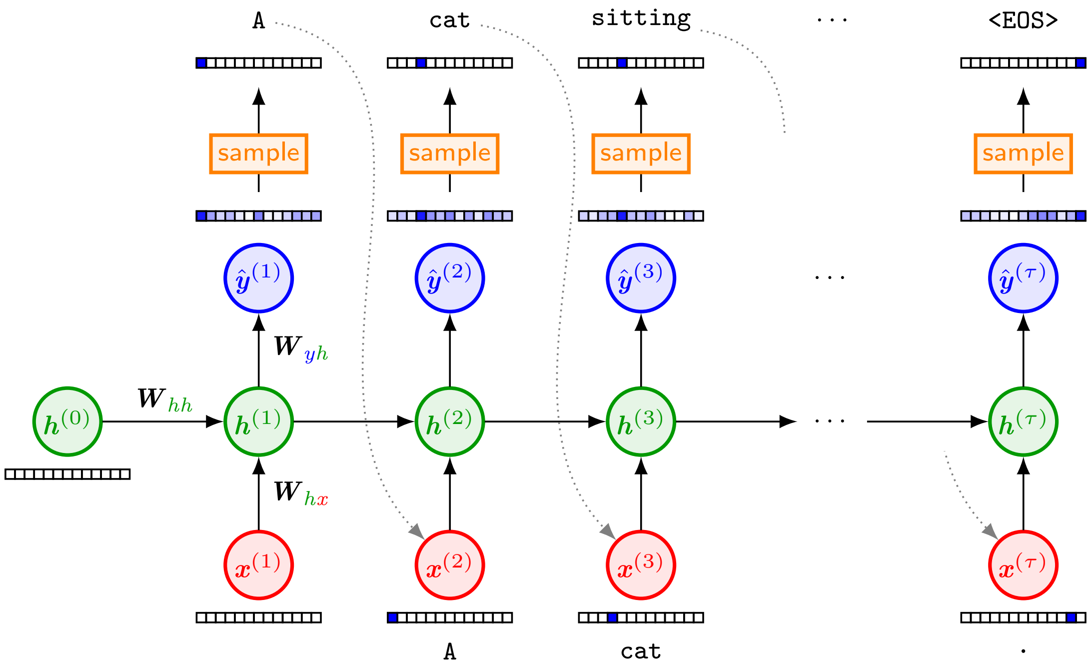
teacher forcing

$$L = \sum_{t=1}^{\tau} L^{(t)} = \sum_{t=1}^{\tau} L(\hat{\boldsymbol{y}}^{(t)}, \boldsymbol{y}^{(t)}) \quad \text{where} \quad L(\hat{\boldsymbol{y}}^{(t)}, \boldsymbol{y}^{(t)}) = -\underbrace{\sum_{i}^{|\text{vocab}|} y_i^{(t)} \log \hat{y}_i^{(t)}}_{\text{cross-entropy loss}}$$

Sampling novel sentences

- use your trained model ($\rightarrow$ you can get a sense of what it has learned)
  - training: $\boldsymbol{x}^{(t)} = \boldsymbol{y}^{(t-1)}$
  - sampling: $\boldsymbol{x}^{(t)} \sim \hat{\boldsymbol{y}}^{(t-1)}$

  $\Bigg\}$ same initialization: $\boldsymbol{x}^{(1)} = \mathbf{0}, \boldsymbol{h}^{(0)} = \mathbf{0}$



- one additional complication:
  - must determine the sequence length τ
  - this can be achieved in various ways

1. a special input symbol (end marker like `<EOS>`)
2. extra output unit (predicts whether to continue or end)
3. extra output unit (predicts length τ directly)

approach #1: end marker

- add a special symbol ("end of sequence")
  - when that symbol is generated, the sampling process stops
- applicable when: the output is a symbol taken from a vocabulary
- in training set
  - insert this symbol as an extra member of the sequence (immediately after $\boldsymbol{x}^{(\tau)}$ in each training example)

approach #2

- introduce an extra output unit (Bernoulli)
  - decides (at each time step) either continue generation or halt generation
  - usually a sigmoid unit trained with cross-entropy loss (end or continue)
- more general than approach #1[5]
  - may be applied to any RNN (*e.g.* that emits a sequence of real numbers)

approach #3

- add an extra output that predicts integer τ
  - based on the decomposition

$$P(\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(\tau)}) = P(\tau) P(\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(\tau)} \mid \tau) \tag{34}$$

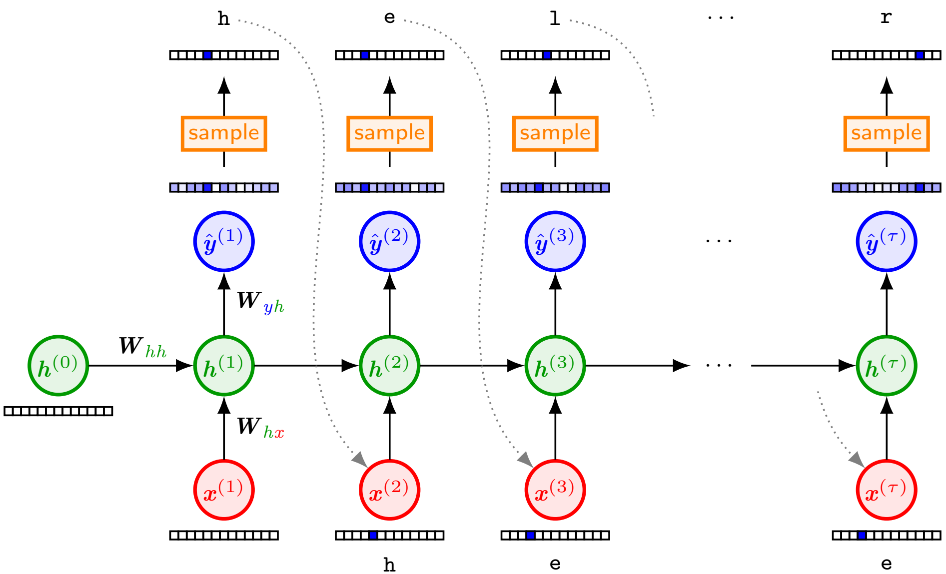
$\Rightarrow$ model can sample a value of τ and then sample τ steps worth of data

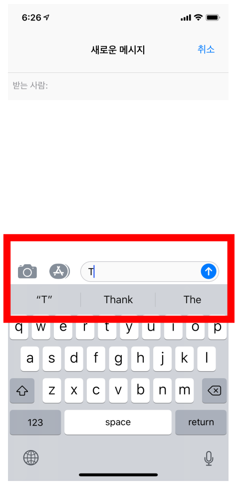
[5] applicable to only RNNs that output a sequence of symbols

Word-level vs character-level

- so far: word-level language modeling
  - vocabulary = [a, aaron, ..., zzz, <UNK>, <EOS>]
- also possible: character -level language modeling
  - vocabulary = [a, b, c, ..., z, ␣, ., ,, ;, ..., 0, 1,..., 9, A, ..., Z]

e.g. sampling 'helicopter'





Example code

- minimal char-level language model (only 112 lines of code) ▸ Link

Instantly share code, notes, and snippets.

karpathy / min-char-rnn.py

Last active 22 hours ago

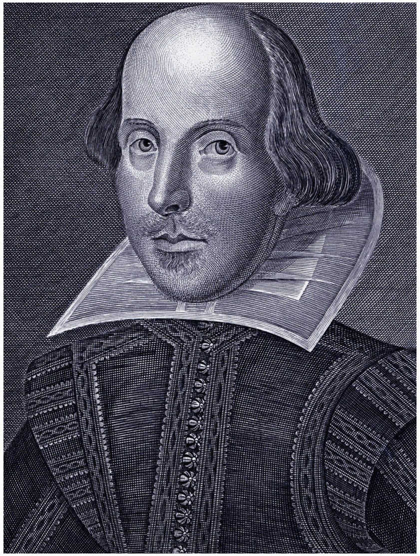
Minimal character-level language model with a Vanilla Recurrent Neural Network, in Python/numpy

min-char-rnn.py

```python
"""
Minimal character-level Vanilla RNN model. Written by Andrej Karpathy (@karpathy)
BSD License
"""
import numpy as np

# data I/O
data = open('input.txt', 'r').read() # should be simple plain text file
chars = list(set(data))
data_size, vocab_size = len(data), len(chars)
print 'data has %d characters, %d unique.' % (data_size, vocab_size)
char_to_ix = { ch:i for i,ch in enumerate(chars) }
ix_to_char = { i:ch for i,ch in enumerate(chars) }

# hyperparameters
hidden_size = 100 # size of hidden layer of neurons
seq_length = 25 # number of steps to unroll the RNN for
learning_rate = 1e-1

# model parameters
Wxh = np.random.randn(hidden_size, vocab_size)*0.01 # input to hidden
Whh = np.random.randn(hidden_size, hidden_size)*0.01 # hidden to hidden
Why = np.random.randn(vocab_size, hidden_size)*0.01 # hidden to output
bh = np.zeros((hidden_size, 1)) # hidden bias
by = np.zeros((vocab_size, 1)) # output bias

def lossFun(inputs, targets, hprev):
  """
  inputs,targets are both list of integers.
  hprev is Hx1 array of initial hidden state
  returns the loss, gradients on model parameters, and last hidden state
  """
  xs, hs, ys, ps = {}, {}, {}, {}
  hs[-1] = np.copy(hprev)
  loss = 0
  # forward pass
  for t in xrange(len(inputs)):
    xs[t] = np.zeros((vocab_size,1)) # encode in 1-of-k representation
    xs[t][inputs[t]] = 1
    hs[t] = np.tanh(np.dot(Wxh, xs[t]) + np.dot(Whh, hs[t-1]) + bh) # hidden state
    ys[t] = np.dot(Why, hs[t]) + by # unnormalized log probabilities for next chars
    ps[t] = np.exp(ys[t]) / np.sum(np.exp(ys[t])) # probabilities for next chars
    loss += -np.log(ps[t][targets[t],0]) # softmax (cross-entropy loss)
  # backward pass: compute gradients going backwards
  dWxh, dWhh, dWhy = np.zeros_like(Wxh), np.zeros_like(Whh), np.zeros_like(Why)
  dbh, dby = np.zeros_like(bh), np.zeros_like(by)
  dhnext = np.zeros_like(hs[0])
  for t in reversed(xrange(len(inputs))):
    dy = np.copy(ps[t])
    dy[targets[t]] -= 1 # backprop into y. see http://cs231n.github.io/neural-networks-case-study/#gra
    dWhy += np.dot(dy, hs[t].T)
    dby += dy
    dh = np.dot(Why.T, dy) + dhnext # backprop into h
    dhraw = (1 - hs[t] * hs[t]) * dh # backprop through tanh nonlinearity
    dbh += dhraw
    dWxh += np.dot(dhraw, xs[t].T)
    dWhh += np.dot(dhraw, hs[t-1].T)
    dhnext = np.dot(Whh.T, dhraw)
  for dparam in [dWxh, dWhh, dWhy, dbh, dby]:
    np.clip(dparam, -5, 5, out=dparam) # clip to mitigate exploding gradients
  return loss, dWxh, dWhh, dWhy, dbh, dby, hs[len(inputs)-1]

def sample(h, seed_ix, n):
  """
  sample a sequence of integers from the model
  h is memory state, seed_ix is seed letter for first time step
  """
  x = np.zeros((vocab_size, 1))
  x[seed_ix] = 1
  ixes = []
  for t in xrange(n):
    h = np.tanh(np.dot(Wxh, x) + np.dot(Whh, h) + bh)
    y = np.dot(Why, h) + by
    p = np.exp(y) / np.sum(np.exp(y))
    ix = np.random.choice(range(vocab_size), p=p.ravel())
    x = np.zeros((vocab_size, 1))
    x[ix] = 1
    ixes.append(ix)
  return ixes

n, p = 0, 0
mWxh, mWhh, mWhy = np.zeros_like(Wxh), np.zeros_like(Whh), np.zeros_like(Why)
mbh, mby = np.zeros_like(bh), np.zeros_like(by) # memory variables for Adagrad
smooth_loss = -np.log(1.0/vocab_size)*seq_length # loss at iteration 0
while True:
  # prepare inputs (we're sweeping from left to right in steps seq_length long)
  if p+seq_length+1 >= len(data) or n == 0:
    hprev = np.zeros((hidden_size,1)) # reset RNN memory
    p = 0 # go from start of data
  inputs = [char_to_ix[ch] for ch in data[p:p+seq_length]]
  targets = [char_to_ix[ch] for ch in data[p+1:p+seq_length+1]]

  # sample from the model now and then
  if n % 100 == 0:
    sample_ix = sample(hprev, inputs[0], 200)
    txt = ''.join(ix_to_char[ix] for ix in sample_ix)
    print '----\n %s \n----' % (txt, )

  # forward seq_length characters through the net and fetch gradient
  loss, dWxh, dWhh, dWhy, dbh, dby, hprev = lossFun(inputs, targets, hprev)
  smooth_loss = smooth_loss * 0.999 + loss * 0.001
  if n % 100 == 0: print 'iter %d, loss: %f' % (n, smooth_loss) # print progress

  # perform parameter update with Adagrad
  for param, dparam, mem in zip([Wxh, Whh, Why, bh, by],
                                [dWxh, dWhh, dWhy, dbh, dby],
                                [mWxh, mWhh, mWhy, mbh, mby]):
    mem += dparam * dparam
    param += -learning_rate * dparam / np.sqrt(mem + 1e-8) # adagrad update

  p += seq_length # move data pointer
  n += 1 # iteration counter
```

code source: Andrej Karpathy. https://gist.github.com/karpathy/d4dee566867f8291f086

- generating Shakespeare-style text



William Shakespeare (1564–1616)

```
tyntd-iafhatawiaoihrdemot lytdws e ,tfti, astai f ogoh eoase
rrranbyne 'nhthnee e plia tklrgd t o idoe ns,smtt h ne etie h,
hregtrs nigtike,aoaenns lng
```

train more

```
"Tmont thithey" fomesscerliund
Keushey. Thom here sheulke,
anmerenith ol sivh I lalterthend Bleipile shuwy fil on aseterlome
coaniogennc Phe lism thond hon at. MeiDimorotion in ther thize."
```

train more

```
Aftair fall unsuch that the hall for Prince Velzonski's that me of
her hearly, and behs to so arwage fiving were to it beloge, pavu say
falling misfort how, and Gogition is so overelical and ofter.
```

train more

```
"Why do what that day," replied Natasha, and wishing to himself
the fact the princess. Princess Mary was easier, fed in had
oftened him. Pierre asking his soul came to the packs and drove up
his father-in-law women.
```

image sources: https://images.app.goo.gl/EDt3MWDdz8vWik3bA; Fei-Fei Li, J. Johnson, S. Yeung, CS231n: Convolutional Neural Networks for Visual Recognition (2017), http://cs231n.stanford.edu/2017/index.html

Application of language modeling: image captioning

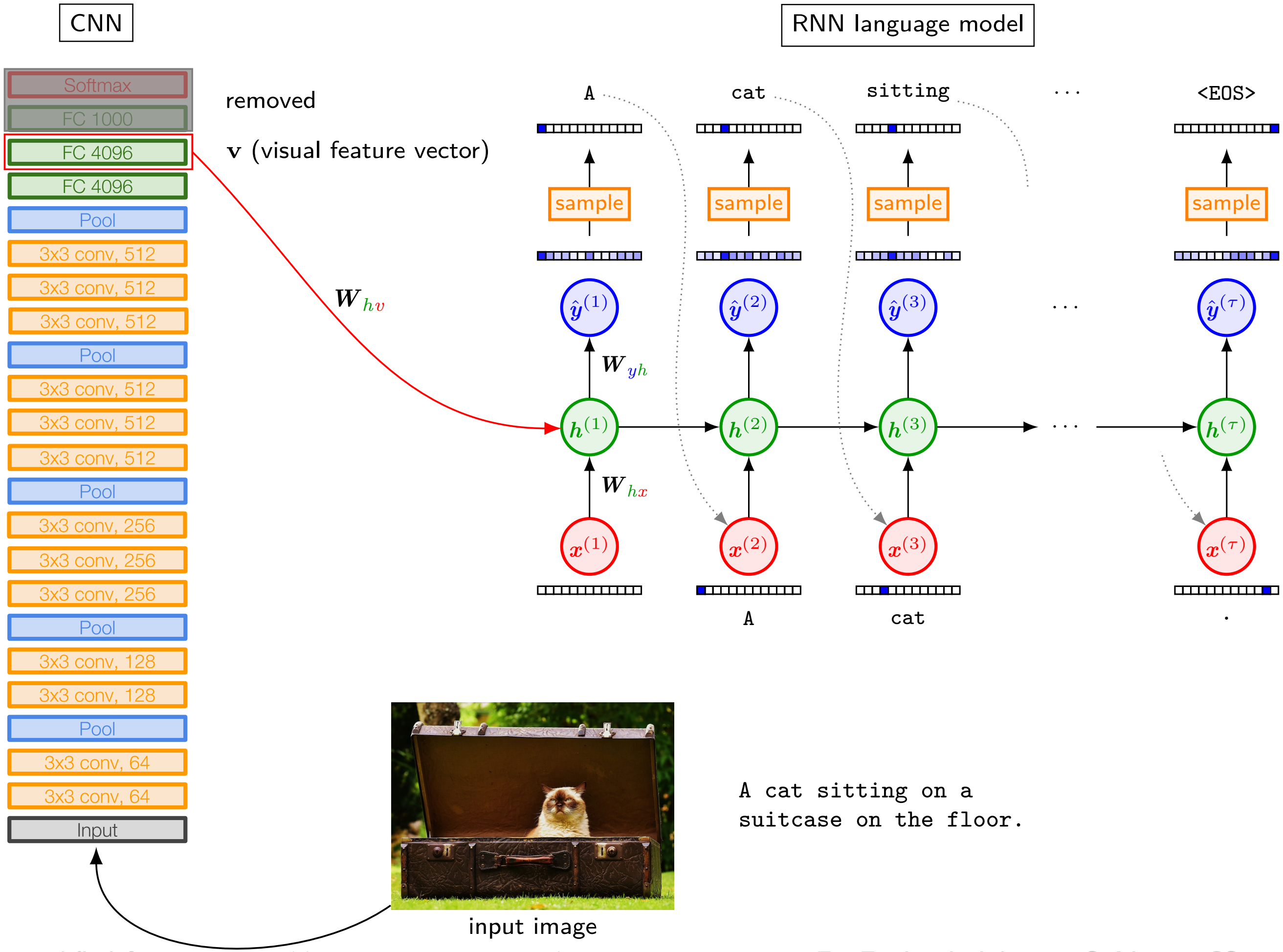


image modified from: https://images.app.goo.gl/3kgPnVqoMVG97Wcx6; Fei-Fei Li, J. Johnson, S. Yeung, CS231n: Convolutional Neural Networks for Visual Recognition (2017), http://cs231n.stanford.edu/2017/index.html

Known heuristics for neural language modeling

1. size matters
   - best models = $\underline{\text{largest}}$ models (esp. # of memory units)
2. regularization matters

   e.g. dropout on input connections
3. CNN vs embedding
   - $\underbrace{\text{character-level CNN models}}_{\uparrow \text{ instead of word embedding}}$ can be used on front-end
4. ensembles matter
   - as usual

source: Rafal Jozefowicz et al. "Exploring the limits of language modeling". In: *arXiv preprint arXiv:1602.02410* (2016)
https://arxiv.org/abs/1602.02410

Outline

Motivation

- all RNNs considered up to now: "Causal" structure

  i.e. state at time t only captures information from

  - past $(\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(t-1)})$ and present input $\boldsymbol{x}^{(t)}$

- but often output $\boldsymbol{y}^{(t)}$ may depend on the *whole input sequence*

  e.g. speech recognition, handwriting recognition, seq-to-seq learning

- speech recognition: correct interpretation of the current sound as a phoneme
  - may depend on next few phonemes (because of co-articulation)

- bidirectional RNN: invented to address that need
  - has been extremely successful

Bidirectional RNN

- learns to map
  - input seq $\boldsymbol{x}$ to target seq $\boldsymbol{y}$ with loss $L^{(t)}$ at each step t
- $\boldsymbol{h}$ recurrence propagates info forward
  - forward in time ($\longrightarrow$)
- $\boldsymbol{g}$ recurrence propagates info backward
  - backward in time ($\longleftarrow$)
- output units $\boldsymbol{o}^{(t)}$ can benefit from
  - a summary of the past in $\boldsymbol{h}^{(t)}$
  - a summary of the future in $\boldsymbol{g}^{(t)}$

$\hat{y}$

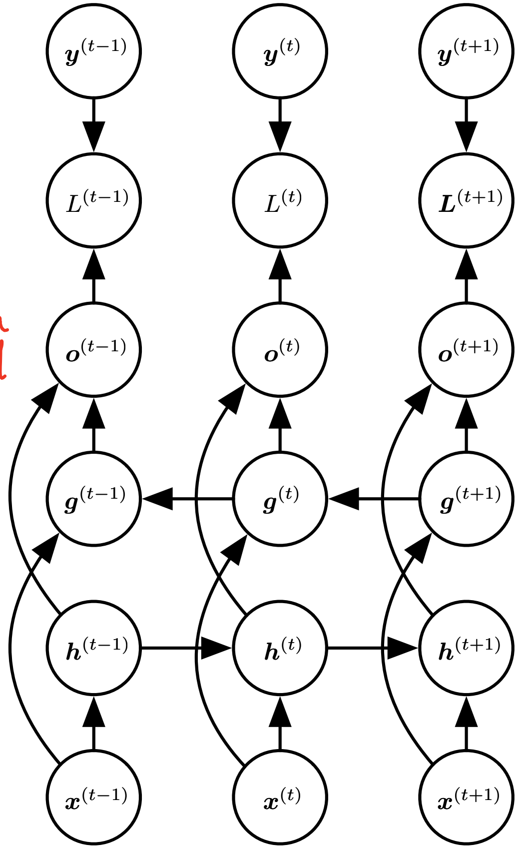


image source: I. Goodfellow, Y. Bengio, and A. Courville, *Deep learning*. MIT Press, 2016

Extension to 2D (*e.g.* images)

- use *four* RNNs: each one goes up, down, left, right
- output $O_{i,j}$ at each point (i, j) can capture
  - mostly local information
  - but also long-range information (if RNN learns to carry that info)
- more expensive than CNN
  - but allow for long-range $\underbrace{\text{lateral interactions}}_{\substack{\uparrow \\ \text{between features in the same feature map}}}$

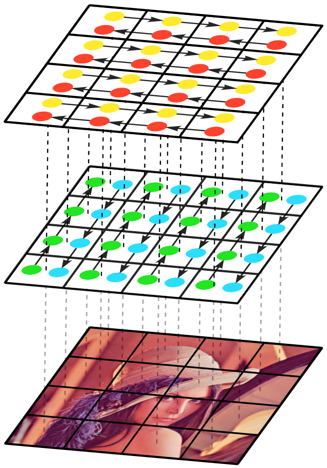


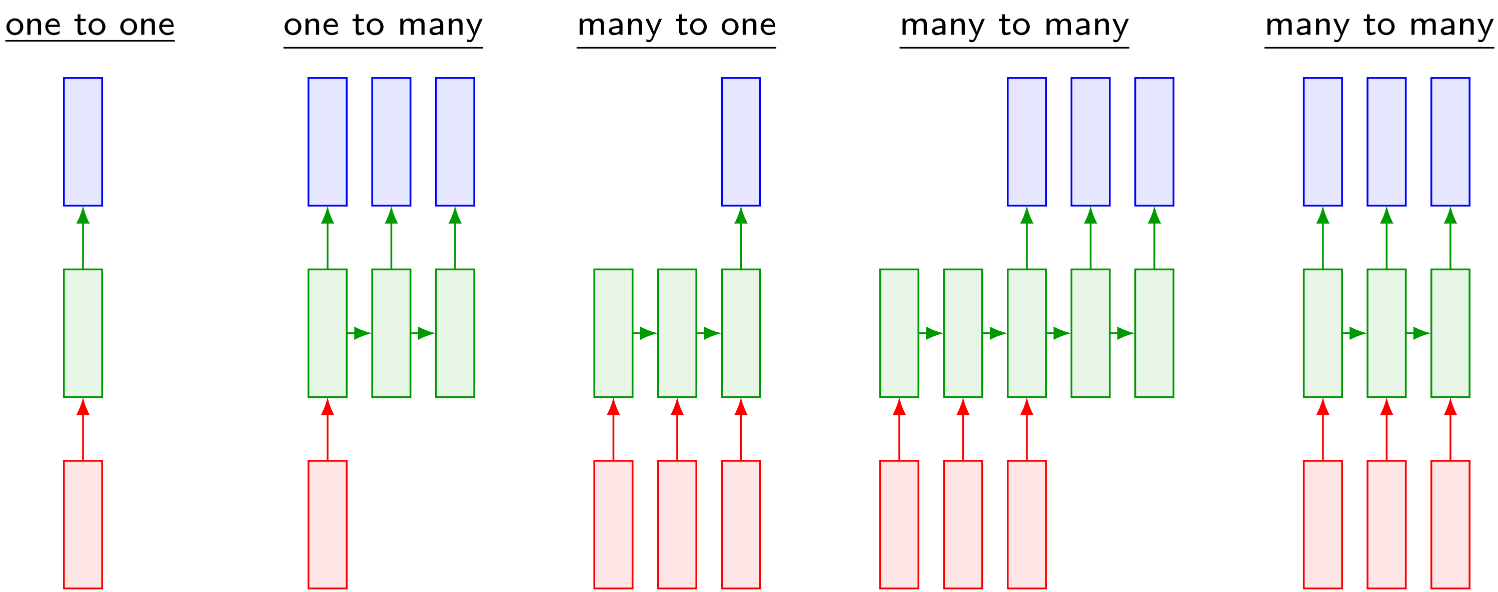
image source: Francesco Visin et al. "ReNet: A recurrent neural network based alternative to convolutional networks". In: *arXiv preprint arXiv:1505.00393* (2015) https://arxiv.org/abs/1505.00393

Outline

Recall: RNN modeling capability

e.g. **image captioning**
image → sentence

e.g. **machine translation**
seq of words → seq of words



vanilla neural net

e.g. **sentiment classification**
sentence → sentiment

e.g. **video frame classification**
seq of frame → seq of class

image source: Fei-Fei Li, J. Johnson, S. Yeung, CS231n: Convolutional Neural Networks for Visual Recognition (2017), `http://cs231n.stanford.edu/2017/index.html`

Mapping sequence to sequence (of different lengths)

- RNN can be trained to map an input sequence to an output sequence
  - which is not necessarily of the same length

- this comes up in many applications

  e.g. speech recognition, machine translation, question answering

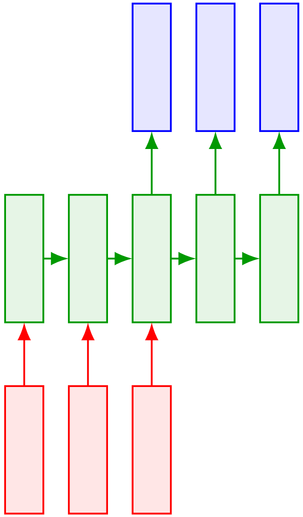
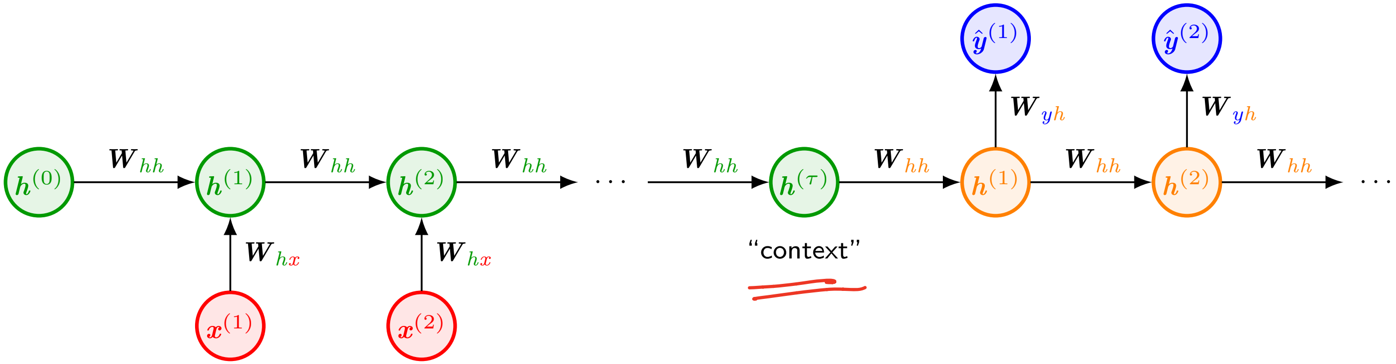


image source: Fei-Fei Li, J. Johnson, S. Yeung, CS231n: Convolutional Neural Networks for Visual Recognition (2017), `http://cs231n.stanford.edu/2017/index.html`

$\boxed{\text{sequence-to-sequence}}$ (= many-to-one + one-to-many)

- many-to-one (encoder)
  - encode input sequence into a single vector
- one-to-many (decoder)
  - produce output sequence from the single input vector

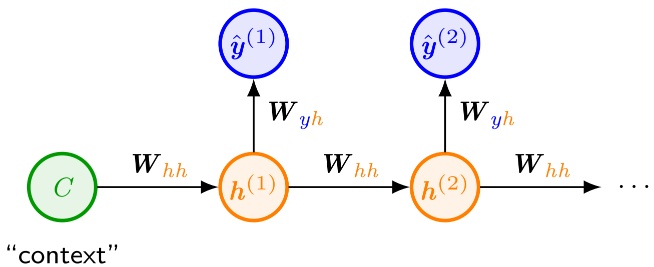


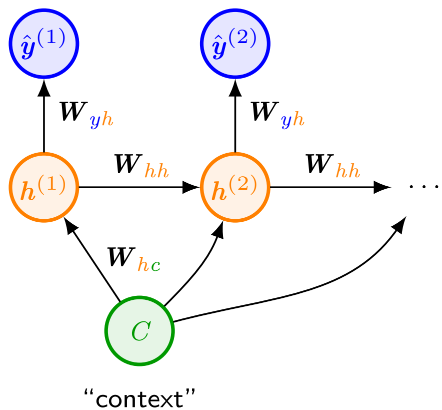
- Context C: a vector (or a sequence of vectors in attention model)
  - summarizes the input sequence $\boldsymbol{X} = (\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(n_x)})$
  - output from the encoder/input to the decoder

Receiving inputs in decoder

- a one-to-many (vector-to-sequence) RNN
  - can receive input in two ways

1. input can be provided as initial state of RNN, or
2. input can be connected to hidden units at each time step





Encoder-decoder/sequence-to-sequence architecture

- goal: map a variable-length sequence to another variable-length sequence
  - first application: machine translation

- two names
  - encoder-decoder architecture (Cho *et al.*, 2014)
  - sequence-to-sequence architecture (Sutskever *et al.*, 2014)

- corresponds to
  - many-to-many RNN

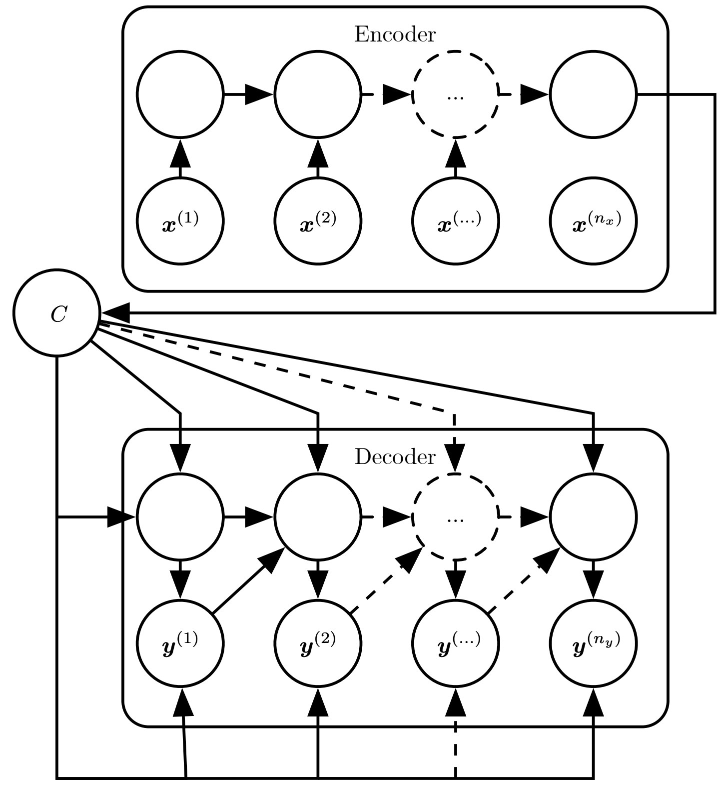
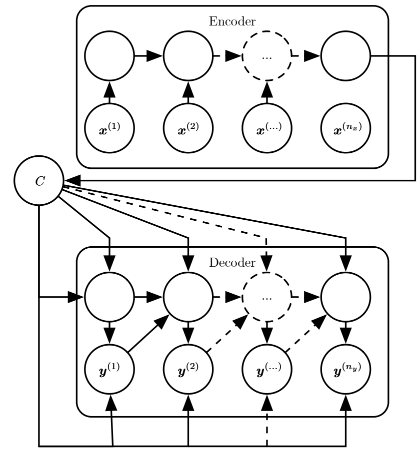


image source: I. Goodfellow, Y. Bengio, and A. Courville, *Deep learning*. MIT Press, 2016

(1) encoder/reader/input RNN:

- processes input sequence $\boldsymbol{X} = (\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(n_x)})$
- emits $\underbrace{\text{context } C}_{\uparrow}$ (generally a fixed-size vector)
  - usually a simple function of final hidden state $\boldsymbol{h}_{n_x}$
  - represents a semantic summary of input seq



(2) decoder/writer/output RNN:

- takes context C as input
- generates output sequence $\boldsymbol{Y} = (\boldsymbol{y}^{(1)}, \ldots, \boldsymbol{y}^{(n_y)})$

- encoder/decoder RNNs: trained jointly
  - to maximize the $\underbrace{\text{average}}_{\uparrow}$ of $\log P(\boldsymbol{y}^{(1)}, \ldots, \boldsymbol{y}^{(n_y)} \mid \boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(n_x)})$

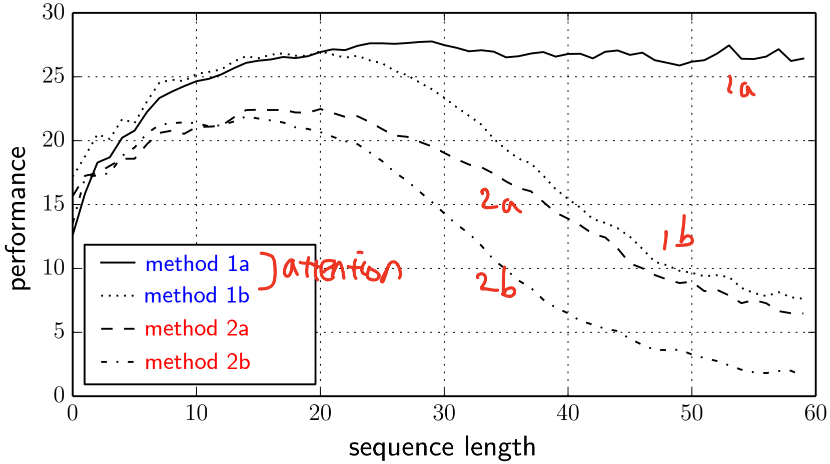
    over all the pairs of $\boldsymbol{X}$ and $\boldsymbol{Y}$ sequences in training set

- innovation of this architecture: not necessarily $n_x = n_y$

image source: I. Goodfellow, Y. Bengio, and A. Courville, *Deep learning*. MIT Press, 2016

Attention mechanism

- one clear limitation
  - dimension of context C may be too small to summarize a long sequence



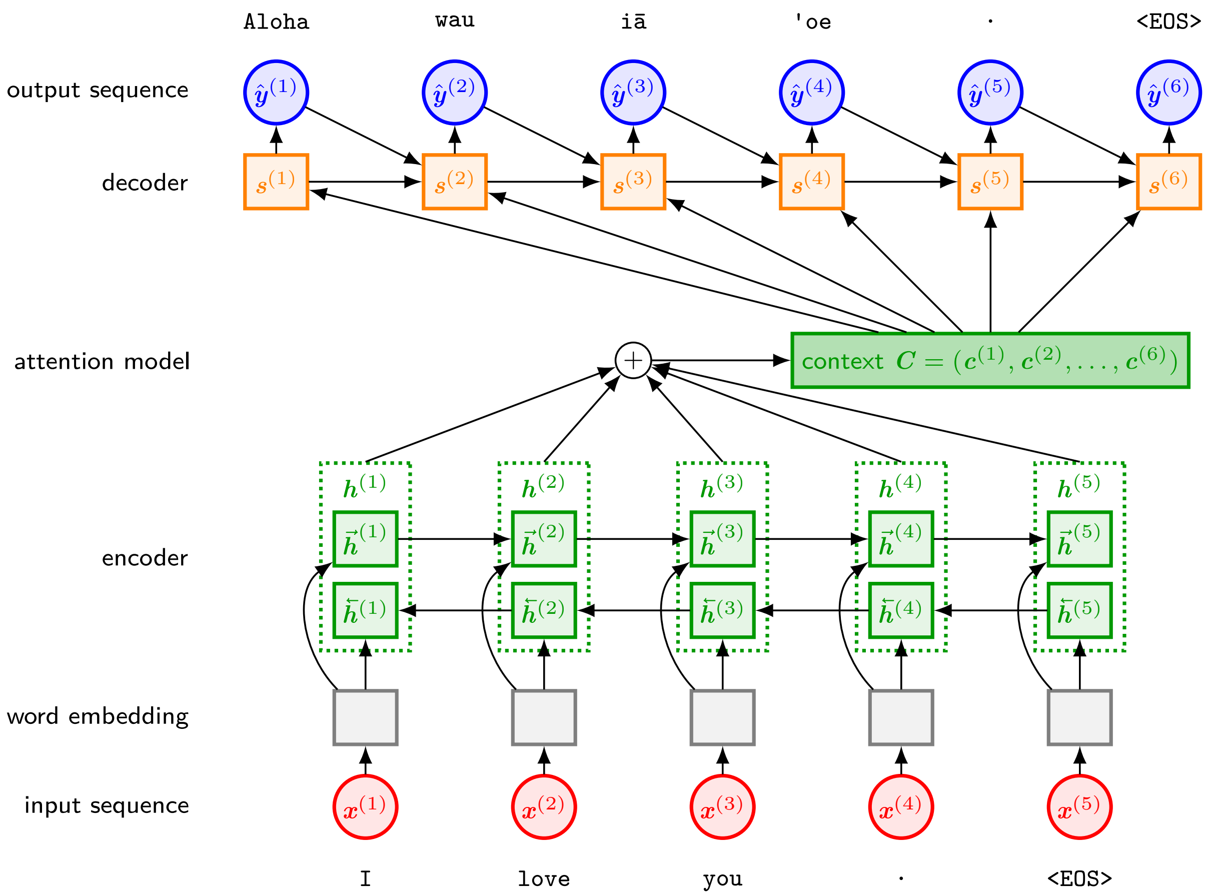
- methods 1 and 2
  - with and without attention, respectively
- a and b
  - trained with max 50 and 30 words, respectively

- attention mechanism
  - makes $\boldsymbol{C}$ a variable-length ~~sequence~~ vector (not a fixed-size vector)
  - learns to associate

$$\text{element } \boldsymbol{c}^{(t)} \text{ of sequence } \boldsymbol{C} \leftrightarrow \text{element } \boldsymbol{y}^{(t)} \text{ of output sequence}$$

image modified from: Dzmitry Bahdanau, Kyunghyun Cho, and Yoshua Bengio. "Neural machine translation by jointly learning to align and translate". In: *arXiv preprint arXiv:1409.0473* (2014) https://arxiv.org/abs/1409.0473

- example



Aloha
wau
iā
'oe
.
<EOS>
output sequence
$\hat{y}^{(1)}$ $\hat{y}^{(2)}$ $\hat{y}^{(3)}$ $\hat{y}^{(4)}$ $\hat{y}^{(5)}$ $\hat{y}^{(6)}$
decoder
$s^{(1)}$ $s^{(2)}$ $s^{(3)}$ $s^{(4)}$ $s^{(5)}$ $s^{(6)}$
attention model
$+$
context $C = (c^{(1)}, c^{(2)}, \ldots, c^{(6)})$
$h^{(1)}$ $h^{(2)}$ $h^{(3)}$ $h^{(4)}$ $h^{(5)}$
encoder
$\vec{h}^{(1)}$ $\vec{h}^{(2)}$ $\vec{h}^{(3)}$ $\vec{h}^{(4)}$ $\vec{h}^{(5)}$
$\overleftarrow{h}^{(1)}$ $\overleftarrow{h}^{(2)}$ $\overleftarrow{h}^{(3)}$ $\overleftarrow{h}^{(4)}$ $\overleftarrow{h}^{(5)}$
word embedding
input sequence
$x^{(1)}$ $x^{(2)}$ $x^{(3)}$ $x^{(4)}$ $x^{(5)}$
I
love
you
.
<EOS>

- more details: Link
  - let $\underbrace{t \in [1, n_y]}_{\substack{\uparrow \\ \text{output index}}}$ and $\underbrace{t' \in [1, n_x]}_{\substack{\uparrow \\ \text{input index}}}$
  - context sequence $\boldsymbol{C} = (\boldsymbol{c}^{(1)}, \boldsymbol{c}^{(2)}, \ldots, \boldsymbol{c}^{(n_y)})$

$$\boldsymbol{c}^{(t)} = \sum_{t'=1}^{n_x} \alpha^{(t,t')} \boldsymbol{h}^{(t')}$$

  - $\alpha^{(t,t')}$: amount of attention $\boldsymbol{y}^{(t)}$ should pay to $\boldsymbol{h}^{(t')}$

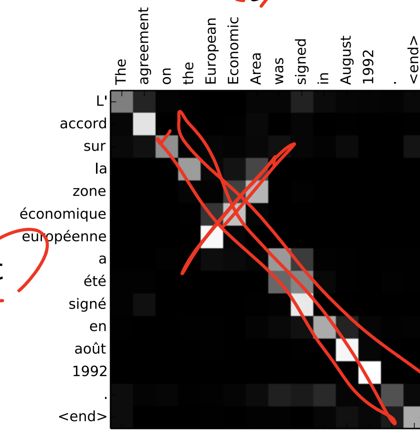
$$\alpha^{(t,t')} = \frac{\exp(e^{(t,t')})}{\sum_{t'=1}^{n_x} \exp(e^{(t,t')})}$$

  - $e^{(t,t')}$: learned by a neural net

$$e^{(t,t')} = f(\boldsymbol{h}^{(t')}, \boldsymbol{s}^{(t-1)})$$

t'

t



$\alpha^{(t,t')}$

Alignment

English $\rightarrow$ French

- t': English
- t: French

image modified from: Dzmitry Bahdanau, Kyunghyun Cho, and Yoshua Bengio. "Neural machine translation by jointly learning to align and translate". In: *arXiv preprint arXiv:1409.0473* (2014) https://arxiv.org/abs/1409.0473

Outline

Computation in most RNNs

- can be decomposed into
  - three blocks of parameters and associated transformations:

1. from input to hidden state ($i \to h$)
2. from previous hidden state to next hidden state ($h \to h$)
3. from hidden state to output ($h \to o$)

- consider a vanilla RNN

- each of these three blocks
  - associated with a single weight matrix

$\Rightarrow$ corresponds to a shallow transformation

$\uparrow$

a learned affine transformation
followed by a fixed nonlinearity
$=$ a single layer in MLP

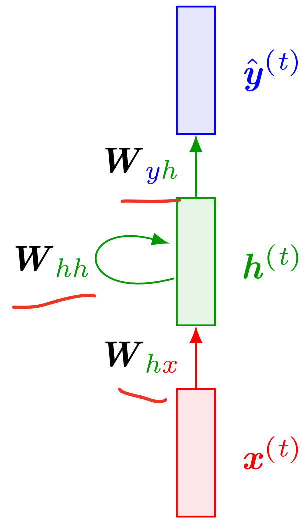
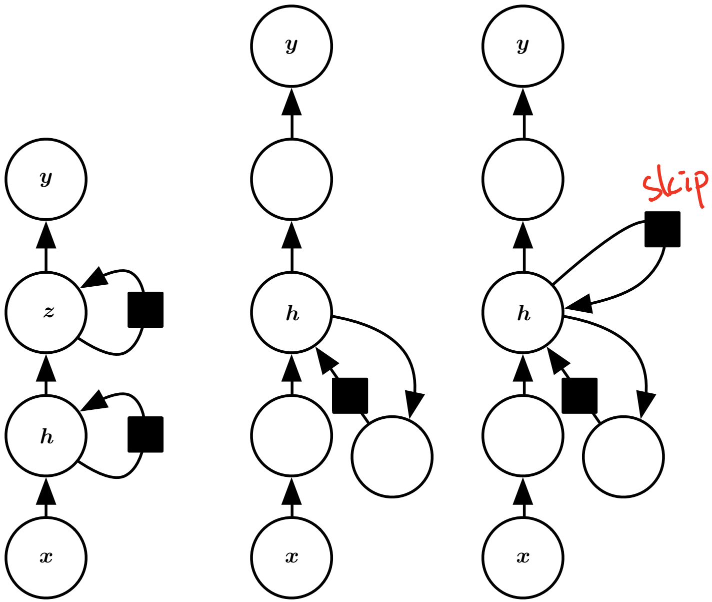


image source: Fei-Fei Li, J. Johnson, S. Yeung, CS231n: Convolutional Neural Networks for Visual Recognition (2017), http://cs231n.stanford.edu/2017/index.html

Deep RNN

- would it be advantageous to introduce depth in each of these operations? $\boxed{\text{yes.}}$



(a) (b) (c)

- three examples:

(a) hidden recurrent state can be broken down
  - into groups organized hierarchically

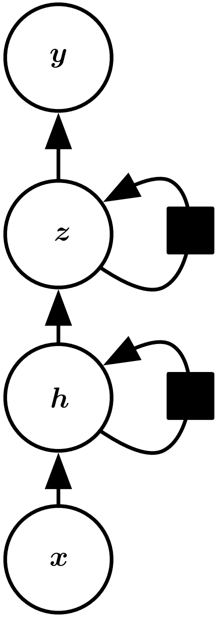
(b) deeper computation (*e.g.* an MLP) can be introduced
  - in input-to-hidden, hidden-to-hidden and hidden-to-output parts
  - this may lengthen shortest path linking different time steps

(c) path-lengthening effect can be mitigated
  - by introducing skip connections

image source: I. Goodfellow, Y. Bengio, and A. Courville, *Deep learning*. MIT Press, 2016

Example (a)

- decompose the hidden state into multiple layers
- lower layer $\rightarrow$ higher layer in hierarchy
  - raw data $\rightarrow$ higher-level representation
- in practice
  - hidden layer depth: not much greater than 2–3



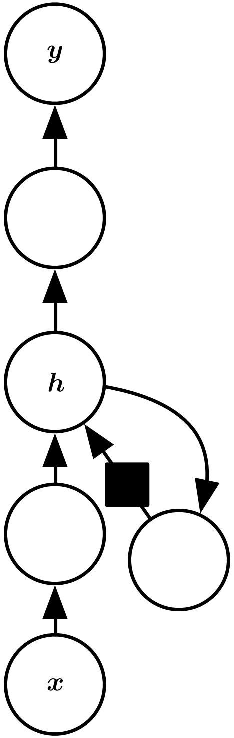
(a)

image source: I. Goodfellow, Y. Bengio, and A. Courville, *Deep learning*. MIT Press, 2016

Example (b)

- we can go a step further from example (a)
  - a separate (deep) MLP for each of the three blocks

- but adding depth
  - may hurt learning by making optimization difficult
  - makes $\underbrace{\text{the shortest path}}_{\substack{\uparrow \\ \text{from a variable in step } t \\ \text{to a variable in step } t+1}}$ become longer

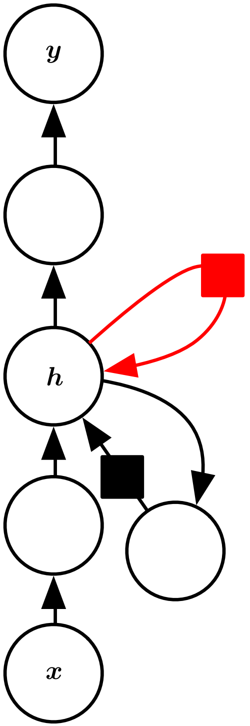


(b)

image source: I. Goodfellow, Y. Bengio, and A. Courville, *Deep learning*. MIT Press, 2016

Example (c)

- path-lengthening can be mitigated by
  - introducing skip connections in hidden-to-hidden path



(c)

image source: I. Goodfellow, Y. Bengio, and A. Courville, *Deep learning*. MIT Press, 2016

Outline

Recursive neural networks[6]

- represent yet another generalization of recurrent nets
  - has potential use for learning to reason
- comparison: computational graph
  - recurrent neural nets: chain-like structure
  - recursive neural nets: structured as a deep tree
- have been successfully applied to
  - processing *data structures* as input to neural nets
  - natural language processing, computer vision

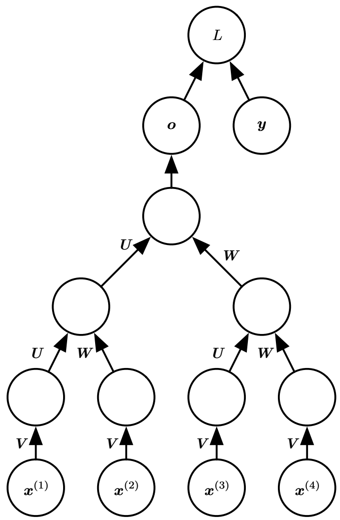


image source: I. Goodfellow, Y. Bengio, and A. Courville, *Deep learning*. MIT Press, 2016

[6] do not abbreviate "recursive neural network" as "RNN" to avoid confusion with "recurrent neural network"

Example

- a variable-size sequence $\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(t)}$
  - can be mapped to a fixed-size representation (output $\boldsymbol{o}$)
  - with fixed parameters (weight matrices $\boldsymbol{U}$, $\boldsymbol{V}$, $\boldsymbol{W}$)
- this figure: supervised learning case
  - $\underbrace{\text{target } \boldsymbol{y}}_{\uparrow}$ is provided

    associated with the whole sequence

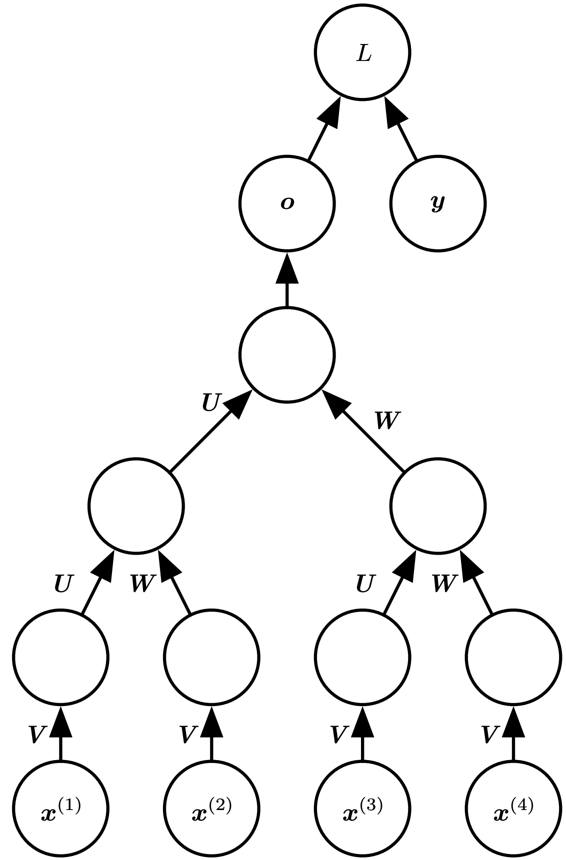


image source: I. Goodfellow, Y. Bengio, and A. Courville, *Deep learning*. MIT Press, 2016

Benefits

- one clear advantage of recursive nets over RNNs:
  - for a sequence of the same length τ,
  - the depth can be drastically reduced from τ to $O(\log \tau)$

    (measured as the number of compositions of nonlinear operations)

  $\Rightarrow$ which might help deal with long-term dependencies

- an open question: how to best structure the tree
- one option: have a tree structure independent of data

  e.g. balanced binary tree

- in some application domains
  - external methods can suggest the appropriate tree structure

  e.g. parse tree provided by natural language parser

Outline

Summary

- sequential data: ubiquitous (speech recognition, machine translation, DNA, ...)
  - examples considered: character-level language modeling, image captioning
- recurrent neural net (RNN): for processing sequential data
  - use recurrence to keep track of the state of a dynamical system
    - hidden-to-hidden: more expressive but slower to train
    - output-to-hidden: less expressive but faster to train
  - training techniques: BPTT (most common), RTRL, teacher forcing
- a variety of RNN structures
  - bidirectional, encoder-decoder/sequence-to-sequence, deep, recursive
- key challenge: vanishing/exploding gradient problems
  - motivated gated RNNs (*e.g.* LSTM and GRU; next lecture)