

M2177.003100 Deep Learning

[8: Recurrent Neural Nets (Part 2)]

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(last compiled at 13:24:00 on 2018/10/21)

Outline

Challenge: Learning Long-Term Dependencies

Gated Recurrent Neural Networks

Summary

References

- Deep Learning by Goodfellow, Bengio and Courville Link
 - ▶ Chapter 10 Sequence Modeling: Recurrent and Recursive Nets
- online resources:
 - ► Understanding LSTM Networks Link
 - The Unreasonable Effectiveness of RNNs Link

 - ► Stanford CS231n: CNN for Visual Recognition Link
 - ► Machine Learning Yearning Link

Challenges in RNN training

- if well trained, RNN can learn dependencies across hundreds of steps!
 - ▶ but very hard to train in practice
- basic problem: gradients propagated over many stages tend to either
 - ▶ vanish (most of the time) or explode는 탐지는 더 쉬움
 - explode (rarely, but with much damage to optimization)

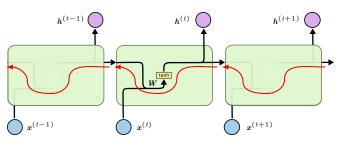
time wise 계속 곱해주기 때문에 vanish/explode 안하려면 값이 1근방 이어야하는 문제점이 있음

- exponentially smaller weights given to long-term interactions
- example: predicting the next word
 - (a) Jane walked into the room. John walked in too. Jane said hi to ______.
 - (b) Jane walked into the room. John walked in too. It was late in the day, and everyone was walking home after a long day at work. Jane said hi to john .

(source: Socher)

Gradient flow in vanilla RNN

- ullet backprop of gradient through the h path involves
- W와 tanh를 여러번 곱해야함
- lacktriangleright many factors of $oldsymbol{W}$ and repeated tanh



(source: cs231n, Olah)

- ullet repeated multiplication of the $^{
 m same}$ W
 - lacktriangledown largest singular value $>1\Rightarrow$ exploding gradients
 - ▶ largest singular value $< 1 \Rightarrow$ vanishing gradients

Analyzing recurrence relation

consider recurrence relation (no activation/input for simplicity)

$$\boldsymbol{h}^{(t)} = \boldsymbol{W}^{\top} \boldsymbol{h}^{(t-1)}$$

simplified to

$$oldsymbol{h}^{(t)} = \left(oldsymbol{W}^t
ight)^{ op} oldsymbol{h}^{(0)}$$

ullet if W admits an eigendecomposition (with orthogonal Q)

$$\pmb{W} = \pmb{Q} \pmb{\Lambda} \, \pmb{Q}^{ op}$$

the recurrence may be simplified further to

$$\boldsymbol{h}^{(t)} = \boldsymbol{Q}^{\top} \boldsymbol{\Lambda}^{t} \boldsymbol{Q} \boldsymbol{h}^{(0)}$$

- ullet each eigenvalue λ : raised to the power of t
 - if $|\lambda| < 1 \Rightarrow$ decay to zero
 - if $|\lambda| > 1 \Rightarrow \text{explode}$
- ullet this problem: particular to RNN (assume scalar weight w for simplicity)
 - (1) RNN: multiply the same weight w by itself many times
 - ightharpoonup product: w^t
 - \Rightarrow vanish or explode depending on magnitude of w
 - (2) non-RNN: use different weight $w^{(t)}$ at each time step
 - ▶ product: $\prod_t w^{(t)}$
 - ⇒ careful scaling can avoid vanishing/exploding¹ to some extent

 $^{^{1}}e.g.$ random $w^{(t)}$ (0 mean, variance v) \rightarrow variance of product: $O(v^{n}) \rightarrow$ set $v = \sqrt[n]{v^{*}}$ (v^{*} : desired bias)

Implications

- exploding gradient
 - ► easy to detect : overflow in gradient computation

 training cannot continue
 - ▶ a quick solution: gradient clipping gradient clipping: 다음슬라이드 참고
- component가 똑똑해서 뭐가 문제 생겨도 계속 진

 vanishing gradient 행해서 발견 자체도 어려움
 - \blacktriangleright can go undetected while drastically $\underbrace{\text{hurting training}}_{\uparrow}$

both learning quality and speed

- heuristic solutions exist (e.g. IRNN)
- more general solution: need to change RNN architecture

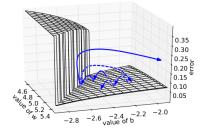
=> LSTM, GRU

Gradient clipping

- a simple solution to exploding gradient
 - ▶ clip gradients to a _____ number whenever they explode

```
grad_norm = np.sum(grad * grad)
if grad norm > threshold:
    grad *= (threshold / grad_norm)
                                                # norm clipping
```

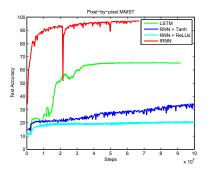
- example: effect of gradient clipping
 - error surface of a single hidden unit RNN
 - solid lines: standard sgd
 - dashes: sgd with clipping

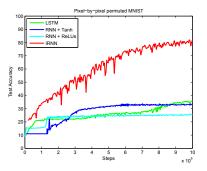


when the standard gradient descent model hits the high error wall, the gradient is pushed off to a faraway location on the decision surface; the clipping model instead pulls back the error gradient to somewhat close to the original gradient landscape (source: Pascanu, 2013)

IRNN (Le, Jaitly & Hinton, 2015)

- a heuristic to handle vanishing gradient
 - 1. initialize W to I (instead of randomly)
 - 2. use ReLU (instead of sigmoid)





Outline

Challenge: Learning Long-Term Dependencies

Gated Recurrent Neural Networks

Long Short-Term Memory (LSTM)
LSTM Variants

Summary

Gated RNNs

very effective sequence models used in practical applications

```
e.g. long short-term memory (LSTM) =>요놈들이 building block(전체 NN의 구조는 별개) gated recurrent unit (GRU)
```

• create paths through time

기존의 RNN에서는 param sharing해서 weight이 time에 independent했는데 이제는 time에 따라 change할 수 있음

▶ these paths have derivatives that neither vanish nor explode W는 time

connection weights may change at each time step

independent하지만 gate action이 time dependent함!!!!

□ not directly but through the action of gates

 $m{W}
ightarrow ext{gates}
ightarrow ext{gradient flow control}$

time-independent time-varyin

 \Rightarrow no repeated multiplication by the same W any more

Idea

- use some units to allow the network to accumulate information
 - ▶ (e.g. evidence for a particular feature or category) over a long duration
- however, once that information has been used
 - ▶ it might be useful for the neural net to forget the old state
- instead of manually deciding when to clear the state
 - we want the neural net to learn to decide when to do it
 - \Rightarrow this is what gated RNNs do!

=>언제 기억하고 언제 forget할 지를 learn 하겠다!

Outline

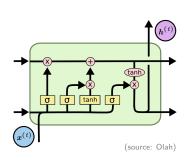
Challenge: Learning Long-Term Dependencies

Gated Recurrent Neural Networks
Long Short-Term Memory (LSTM)

Summary

LSTM (Hochreiter and Schmidhuber, 1997) LSTM도 revision이 많음 => initial부터 쭉 알아보자!

- a core contribution of initial LSTM:
 - > use self-loops to produce paths where gradient can flow for long durations
 vanilla rnn unit을 LSTM으로 drop and
 replace 가능 => input/output interface가
- e a crucial addition: make weight on this self-loop খণ্ণই
 - conditioned on the context rather than fixed
 - " gated " (i.e. controlled by another hidden unit)
 - gating action changes dynamically (based on input)
 - extremely successful in many applications:
 - handwriting recognition
 - speech recognition
 - handwriting generation
 - machine translation
 - image captioning
 - many more!



gate는 time dependent! gate의 weight는 time

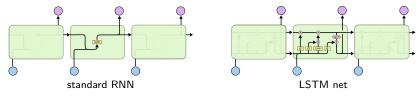
indepent...

LSTM networks

- explicitly designed to avoid long-term dependency problem
 - lacktriangleright remembering info for long time: practically their $\underline{\underline{}^{ ext{default}}}$ behavior
- standard RNNs: a chain of repeating modules

 very simple structure (single tanh layer)
- LSTMs: also a chain of repeating modules

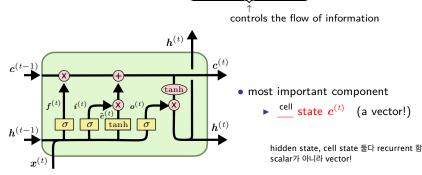
more complex (four interacting network layers)



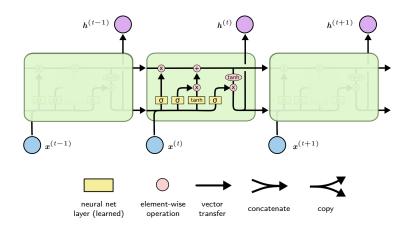
(source: Olah)

LSTM cells

- LSTM RNNs consists of "LSTM cells"
 - ▶ have an internal recurrence (a self-loop) besides the outer recurrence
- each LSTM cell: has the same inputs/outputs as in standard RNN
 - but has more parameters and a system of gating units



Notation and conventions



- ▶ each line carries a vector sigmoid => 수도꼭지
- $m \sigma(\cdot)$: for controlling gates tanh => 정보 $m (0 \le \sigma \le 1)$
- ▶ $tanh(\cdot)$: for representing cell state values $(-1 \le tanh \le 1)$

- simplified notation
 - combine hidden-hidden and input-hidden weight matrices

$$egin{aligned} oldsymbol{h}^{(t)} &= g(oldsymbol{W}_{hh}oldsymbol{h}^{(t-1)} + oldsymbol{W}_{hx}oldsymbol{x}^{(t)} + oldsymbol{b}_h) \ & riangleq g(oldsymbol{W}_{h}[oldsymbol{h}^{(t-1)}, oldsymbol{x}^{(t)}] + oldsymbol{b}_h) \end{aligned}$$

where

$$egin{aligned} oldsymbol{W}_h & \triangleq \left[egin{array}{c} oldsymbol{W}_{hh} & oldsymbol{W}_{hx}
ight] \in \mathbb{R}^{n_h imes (n_h + n_x)} \ \left[oldsymbol{h}^{(t-1)}, oldsymbol{x}^{(t)}
ight] & \in \mathbb{R}^{(n_h + n_x) imes 1} \end{aligned}$$

and

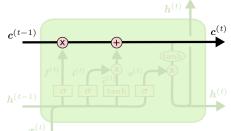
$$egin{aligned} oldsymbol{W}_h[oldsymbol{h}^{(t-1)},oldsymbol{x}^{(t)}] &= [oldsymbol{W}_{hh} oldsymbol{W}_{hx}] egin{bmatrix} oldsymbol{h}^{(t-1)} \ oldsymbol{x}^{(t)} \end{bmatrix} \ &= oldsymbol{W}_{hh}oldsymbol{h}^{(t-1)} + oldsymbol{W}_{hx}oldsymbol{x}^{(t)} \end{aligned}$$

Core idea behind LSTM

- key: cell state
 - like a conveyor belt
 - runs down the entire chain (with only minor linear interactions)
 - \Rightarrow information easily can just flow along the chain unchanged

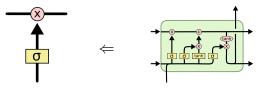
cell state의 각각의 value는

- each element in cell state TIETOUTH
 - ≈ scalar integer counter
 - incremented/decremented by up to one at each time step

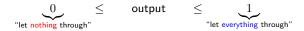


- LSTM can remove/add information to cell state
 - carefully regulated by structures called gates

- gates: a way to optionally let information through
 - composed of
 - ▷ a sigmoid neural net layer
 - ▷ an element-wise multiplication operation



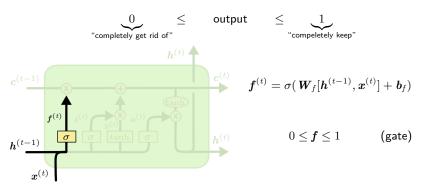
- the sigmoid layer
 - describes how much of each element should be let through
 - outputs a number between zero and one



• standard LSTM: has three gates (forget, input, output)

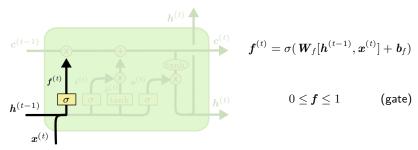
Step 1

- decide what information to throw away from cell state
 - ▶ implemented by a sigmoid layer called forget gate
- ullet forget gate: for each number in cell state $c^{(t-1)}$
 - ▶ looks at $h^{(t-1)}$ and $x^{(t)}$
 - outputs a number between zero and one



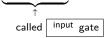
example: language modeling

- predict the next word based on all the previous ones
- cell state
 - might include the gender of the present subject
 - so that the correct pronouns can be used
- when we see a new subject
 - we want to forget the gender of the old subject



Step 2

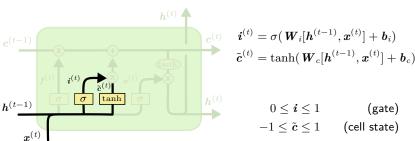
- decide what new information to store in cell state in two substeps
 - (i) a sigmoid layer decides which values to update



(ii) a tanh layer creates a vector of new candidate values

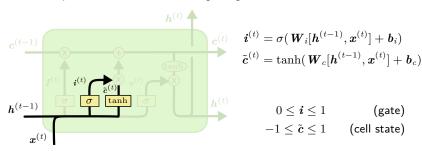
called $ilde{c}^{(t)}$, which could be added to the state

* step 3 will combine these two to create an update to the state



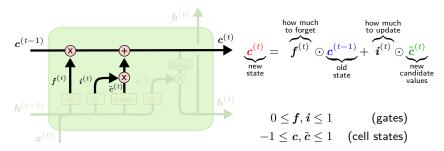
example: language modeling (continued)

- we would want to add the gender of the new subject to cell state
 - ▶ to replace the old one we are forgetting



Step 3

- ullet now it's time to update old cell state $oldsymbol{c}^{(t-1)}$ into new cell state $oldsymbol{c}^{(t)}$
 - ightharpoonup step 2 already decided what to do ightharpoonup we just need to actually do it now

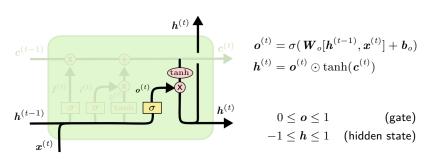


example: language modeling (continued)

- we would actually drop the info about the old subject's gender
 - ▶ and add the new info as decided in step 2

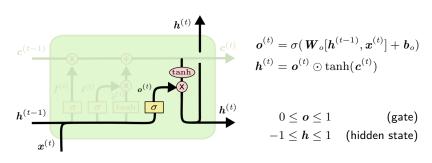
Step 4

- decide what to output ← based on cell state, but will be a filtered version
 - (i) run a sigmoid layer to decide what parts of cell state to output called output gate
 - (ii) put cell state through tanh and multiply it by output gate
 - ⇒ we only output the parts we decided to



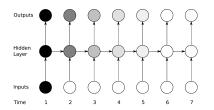
example: language modeling (continued)

- the model just saw a subject
 - it might want to output info relevant to a matching verb
 - e.g. the subject is singular/plural



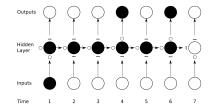
Comparison

vanishing gradient (RNN)



The shading of the nodes in the unfolded network indicates their sensitivity to the inputs at time one (the darker the shade, the greater the sensitivity). The sensitivity decays over time as new inputs overwrite the activations of the hidden layer, and the network forgets the first inputs.

preservation of gradient (LSTM)

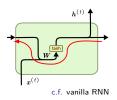


The black nodes are maximally sensitive and the white nodes are entirely insensitive. The state of the input, forget, and output gates are displayed below, to the left and above the hidden layer respectively. For simplicity, all gates are either entirely open (0) or closed (–). The memory cell 'remembers' the first input as long as the forget gate is open and the input gate is closed. The sensitivity of the output layer can be switched on and off by the output gate without affecting the cell

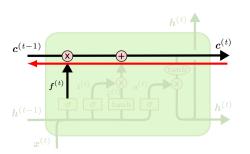
source: Graves (2012)

Gradient flow in LSTM

- ullet backpropagation from $oldsymbol{c}^{(t)}$ to $oldsymbol{c}^{(t-1)}$ involves
 - only element-wise multiplication by f
 - lacktriangleright no matrix multiplication by $oldsymbol{W}$



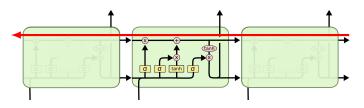
- much nicer than standard RNN for two reasons
 - 1. element-wise multiplication: more efficient than full matrix multiplication



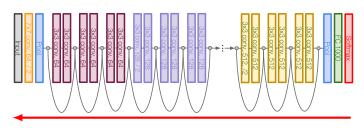
- 2. multiplication by forget gate

 potentially different
 values at every time step
- c.f. vanilla RNN: same W
 - ⇒ more likely to have vanishing/exploding gradient

• backprop through cell state: gradient super highway

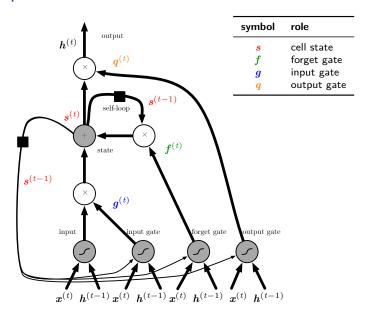


• similar to the effect of skip connections in ResNet

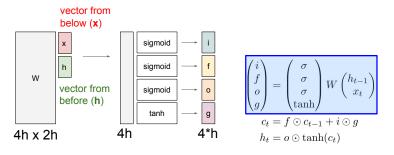


Alternative presentations

textbook



• cs231n



symbol	name	role
\boldsymbol{i}	input gate	whether to write to cell
f	forget gate	whether to erase cell
o	output gate	how much to reveal cell
\boldsymbol{g}	gate gate	how much to write to cell (i.e. new $\frac{candidate}{}$ values $ ilde{c}^{(t)}$)

Outline

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Gated Recurrent Neural Networks

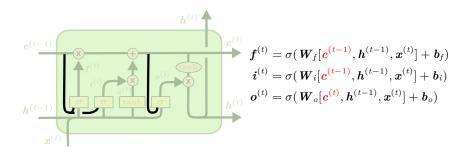
Long Short-Term Memory (LSTM)

LSTM Variants

Summary

Peephole connections

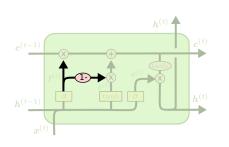
- · make the gate layers look at cell state
 - i.e. use cell state as extra input to gates
 - need additional parameters



 actual peephole connections may vary from architecture to architecture (e.g. see page 32)

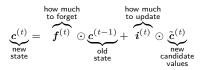
Coupling forget/input gates forget / update 2th 모델

- previously: separate decisions about what to forget and what to update
 forget gate input gate
- now: make these decisions together
 - how much to update = how much to not forget



forget과 update가 independent

• recall: cell state update



forget과 update가 dependent

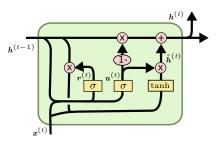
coupled gating

$$c^{(t)} = f^{(t)} \odot c^{(t-1)} + (1 - f^{(t)}) \odot \tilde{c}^{(t)}$$

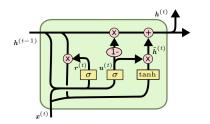
Gated recurrent unit (GRU) (Cho et al., 2014)

GRU => LSTM이 복잡하니까 줄여서 해보자

- major changes over LSTM: simplification
 - combines forget and input gates into a single "update gate"
 - introduces "reset gate"
 - merges cell state and hidden state into one state
- potential advantages over LSTM
 - ▶ fewer _____ ⇒ sometimes easier training/better performance 항상 빠르고 좋은것은 아님! 둘다 해봐야함!



$$\begin{aligned} & \boldsymbol{u}^{(t)} = \sigma(\boldsymbol{W}_{u}[\boldsymbol{h}^{(t-1)}, \boldsymbol{x}^{(t)}]) \\ & \boldsymbol{r}^{(t)} = \sigma(\boldsymbol{W}_{r}[\boldsymbol{h}^{(t-1)}, \boldsymbol{x}^{(t)}]) \\ & \tilde{\boldsymbol{h}}^{(t)} = \tanh(\boldsymbol{W}[\boldsymbol{r}^{(t)} \odot \boldsymbol{h}^{(t-1)}, \boldsymbol{x}^{(t)}]) \\ & \boldsymbol{h}^{(t)} = (1 - \boldsymbol{u}^{(t)}) \odot \boldsymbol{h}^{(t-1)} + \boldsymbol{u}^{(t)} \odot \tilde{\boldsymbol{h}}^{(t)} \end{aligned}$$



$$\mathbf{u}^{(t)} = \sigma(\mathbf{W}_{u}[\mathbf{h}^{(t-1)}, \mathbf{x}^{(t)}])$$
 (1)

$$\mathbf{r}^{(t)} = \sigma(\mathbf{W}_r[\mathbf{h}^{(t-1)}, \mathbf{x}^{(t)}]) \tag{2}$$

$$\tilde{\boldsymbol{h}}^{(t)} = \tanh(\boldsymbol{W}[\boldsymbol{r}^{(t)} \odot \boldsymbol{h}^{(t-1)}, \boldsymbol{x}^{(t)}])$$
 (3)

$$h^{(t)} = (1 - u^{(t)}) \odot h^{(t-1)} + u^{(t)} \odot \tilde{h}^{(t)}$$
 (4)

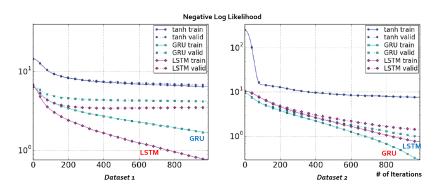
eq	meaning
(1)	update gate $oldsymbol{u}^{(t)}$ is learned from old state $oldsymbol{h}^{(t-1)}$ and current input $oldsymbol{x}^{(t)}$
(2)	reset gate $m{r}^{(t)}$ is learned from old state $m{h}^{(t-1)}$ and current input $m{x}^{(t)}$
(3)	• new candidate value $\tilde{\pmb{h}}^{(t)}$ reflects old state $\pmb{h}^{(t-1)}$ and current input $\pmb{x}^{(t)}$ • reset gate $\pmb{r}^{(t)}$ controls how much old state $\pmb{h}^{(t-1)}$ is used • current input $\pmb{x}^{(t)}$ is fully used regardless of $\pmb{r}^{(t)}$
(4)	• current state $m{h}^{(t)}$ combines old state $m{h}^{(t-1)}$ and new candidate value $\tilde{m{h}}^{(t)}$ • update gate $m{u}^{(t)}$ controls how to $^{ ext{mix}}$ these two

Variants and comparisons

- many more variants of LSTM can be designed
- however, several investigations found
 - ▶ no variant would clearly beat both of LSTM/GRU across a wide range of tasks (Greff et al., 2015; Jozefowicz et al., 2015)
- Greff et al. (2015) found:
 - ▶ a crucial ingredient is the forget gate => forget gate가 매우 중요하다
- Jozefowicz et al. (2015) found:
 - adding a bias of 1 to LSTM forget gate
 - → makes LSTM as strong as the best of explored architectural variants

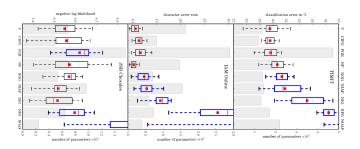
"No clear winner" (Chung, 2014)

but GRU/LSTM-RNNs certainly outperform traditional RNNs



LSTM: a search space odyssey (Greff, 2015)

- large-scale analysis of eight LSTM variants
 - speech/handwriting recognition, polyphonic music modeling
 - ▶ 5400 experimental runs (≈ 15 years of CPU time)
- result: "no variants can improve on standard LSTM significantly"
 - ▶ most critical: forget gate & output activation function

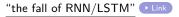


Toward optimal RNN architectures (Jozefowicz, 2015)

- objectives
 - determine whether LSTM is optimal or better one exists
 - better understand the role of individual components
- results from evaluating over 10,000 different architectures
 - found an architecture that outperforms LSTM/GRU
 - fine print: "on some but not all tasks"
- another finding: adding a bias of _____ to LSTM forget gate
 - closes the gap between LSTM and GRU

Outlook

- memory-augmented neural net (MANN)
 - memory networks: learn Q&A tasks
 - neural Turing machines: learn algorithms



- critical problems of RNN/LSTM
 - often very difficult to train
 - hardware acceleration issue: memory-bandwidth bound
- (arguably better) alternatives
 - temporal convolutional networks (TCN) Link
 - ▶ pervasive attention (2D CNN for seq-to-seq prediction) ▶ Link
 - the Transformer (machine translation with self-attention; no RNN/CNN)



Outline

Challenge: Learning Long-Term Dependencies

Gated Recurrent Neural Networks

Summary

Summary

RNN => 트레이닝 잘하면 좋은 결과 나올 수 있지만 트레이 닝 자체가 굉장히 어려움(잘 안되는 경우가 많음)

- challenge of training RNN: learning long-term dependency
 - main cause: vanishing gradient and/or exploding gradient
 - heuristic solutions: gradient clipping, IRNN (limited applicability)
 - ▶ generic solution requires changes in architecture ⇒ gated RNN
- gated RNN: long short-term memory (LSTM), gated recurrent unit (GRU)
 - create paths through time without vanishing/exploding gradients
 - ▶ gates: control how much "open" the signal flows $(0 \le \sigma \le 1)$
 - ▶ cell state: stores system state like a counter $(-1 \le \tanh \le 1)$
 - backprop path through cell state: mainly element-wise multiplication
 - ⇒ helpful to maintain strong gradient flows (similar to ResNet idea)
- further extensions and recent criticism
 - ▶ memory-augmented neural nets: learn Q&A tasks or algorithms
 - ▶ "attention is all you need"