

Deep Natural Language Processing

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Natural Language Processing Tasks (1)

Too many of them here we list a few of what is going on in our lab:

- ▶ **machine translation:** *encoder to decoder*
automatically translate text from one human language to another, for example, English to Chinese. Since 2014, Neural Machine Translation (NMT) dominates!
- ▶ **text summerization:** *context to decoder*
 1. **Extraction-based summarization** extracts objects (part-sentences or words) form the long document without modification, i.e., pick the important bits
 2. **abstraction-based summarization**
involves paraphrasing sections of the source document
- ▶ **Q and A:** *encoder to decoder given context*
the above three (3) may share a design architecture/elements

Natural Language Processing Tasks (2)

Too many of them here we list a few of what is going on in our lab:

- ▶ **natural language generation** by learning document corpus
generate natural language from a machine representation, or for machine to generate semantically-similar texts given a training corpus
- ▶ **chatbot**
enable human and machine to communicate using natural language
- ▶ **natural language to cross-domain translation**
 1. NLP to image
 2. NLP to animation
- ▶ **topic modeling**
this is **unsupervised learning**, tries to assign each document in the document corpus a latent distribution of topics
- ▶ Before we get into it, let's study the foundation of Deep NLP: Recurrent Neural Networks
- ▶ before 2018, it is the primary design element of any D-NLP!

Recurrent Neural Networks

- ▶ RNN equations are simple, it has three sets of parameters: (W , V , U)

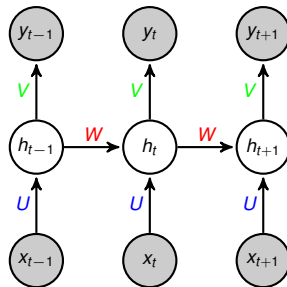
$$h_t = \tanh(\underbrace{Ux_t + Wh_{t-1}}_{z_t}) \quad \hat{y}_t = \text{softmax}(Vh_t)$$

- ▶ The overall loss can be defined as sum of **cross entropy**:

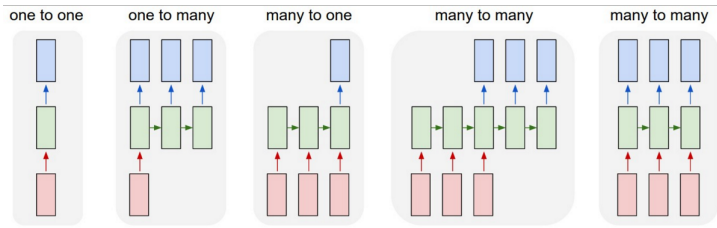
$$C(y, \hat{y}) = \sum_t C_t(y_t, \hat{y}_t) = - \sum_t \underbrace{\sum_{i \in \mathbb{S}} y_{t,i} \log \hat{y}_{t,i}}_{\text{-ve of cross entropy loss}}$$

- ▶ The overall loss can also be defined as sum of **square error**:

$$C(y, \hat{y}) = \sum_t C_t(y_t, \hat{y}_t) = \sum_t \sum_{i \in \mathbb{S}} (y_{t,i} - \hat{y}_{t,i})^2$$



Various applications of RNNs



- ▶ each configuration serves a different applications
- ▶ let's discuss about the scenarios for their use

$$h_t = \tanh(\underbrace{Ux_t + Wh_{t-1}}_{z_t}) \qquad \hat{y}_t = \text{softmax}(\underbrace{Vh_t}_{b_t})$$

$$\mathcal{C}(y, \hat{y}) = \sum_t \mathcal{C}_t(y_t, \hat{y}_t) = - \sum_t \sum_{\mathbb{S}} y_t \log \hat{y}_t$$

where \mathbb{S} is the output space, e.g., all the words we try to predict.

$$\begin{aligned} \frac{\partial \mathcal{C}_t(y_t, \hat{y}_t)}{\partial V} &= \frac{\partial \mathcal{C}_t(y_t, \hat{y}_t)}{\partial b_t} \frac{\partial b_t}{\partial V} \\ &= \frac{\partial (-\sum_{\mathbb{S}} y_t \log \hat{y}_t)}{\partial b_t} \times \underbrace{\frac{\partial b_t}{\partial V}}_{\text{a vector}} \\ &= (\hat{y}_t - y_t) h_t^\top \end{aligned}$$

Back propagation for $\frac{\partial \mathcal{C}_t}{\partial W}$

$$h_t = \tanh(\underbrace{Ux_t + Wh_{t-1}}_{z_t}) \quad \hat{y}_t = \text{softmax}(\underbrace{Vh_t}_{b_t})$$

$$\mathcal{C}(y, \hat{y}) = \sum_t \mathcal{C}_t(y_t, \hat{y}_t) = - \sum_t \sum_{\mathbb{S}} y_t \log \hat{y}_t$$

- ▶ Looking at **individual** cost term \mathcal{C}_t :

$$\frac{\partial \mathcal{C}_t}{\partial W} = \left(\frac{\partial \mathcal{C}_t}{\partial \hat{y}_t} \frac{\partial \hat{y}_t}{\partial h_t} \right) \frac{\partial h_t}{\partial W} = \left(\frac{\partial \mathcal{C}_t}{\partial \hat{y}_t} \frac{\partial \hat{y}_t}{\partial h_t} \right) \sum_{k=0}^t \frac{\partial h_t}{\partial h_k} \frac{\partial h_k}{\partial W}$$

- ▶ when performing $\frac{\partial h_t}{\partial W}$, we need to **sum** over all intermediate latent nodes, i.e.,

$$\left(\frac{\partial h_t}{\partial h_1} \frac{\partial h_1}{\partial W} \right) + \left(\frac{\partial h_t}{\partial h_2} \frac{\partial h_2}{\partial W} \right) + \cdots + \left(\frac{\partial h_t}{\partial h_{t-1}} \frac{\partial h_{t-1}}{\partial W} \right)$$

- ▶ rewrite it to fill in the gap with chain rule:

$$\frac{\partial \mathcal{C}_t}{\partial W} = \sum_{k=0}^t \frac{\partial \mathcal{C}_t}{\partial \hat{y}_t} \frac{\partial \hat{y}_t}{\partial h_t} \left(\prod_{j=k+1}^t \frac{\partial h_j}{\partial h_{j-1}} \right) \frac{\partial h_k}{\partial W}$$

- ▶ we need to sum over all \mathcal{C}_t

Back propagation for $\frac{\partial \mathcal{C}_t}{\partial W}$ (1)

$$h_t = \tanh(\underbrace{Ux_t + Wh_{t-1}}_{z_t}) \quad \hat{y}_t = \text{softmax}(Vh_t)$$

$$\begin{aligned} \frac{\partial \mathcal{C}_t}{\partial W} &= \sum_{k=0}^t \frac{\partial \mathcal{C}_t}{\partial \hat{y}_t} \frac{\partial \hat{y}_t}{\partial h_t} \left(\prod_{j=k+1}^t \frac{\partial h_j}{\partial h_{j-1}} \right) \frac{\partial h_k}{\partial W} \\ &= \sum_{k=0}^t \frac{\partial \mathcal{C}_t}{\partial \hat{y}_t} \frac{\partial \hat{y}_t}{\partial h_t} \left(\prod_{j=k+1}^t \frac{\partial h_j}{\partial h_{j-1}} \right) \frac{\partial h_k}{\partial z_k} \frac{\partial z_k}{\partial W} \end{aligned}$$

► The following has $t + 1$ term, each with varying length due to the product term.

► Derivations can be understood better: $h_2 \left(\underbrace{c_2 + W(h_1(c_1 + W))}_{z_2} \right)$

$$\begin{aligned} &\frac{\partial h_2(c_2 + W(h_1(c_1 + W)))}{\partial W} \\ &= h'_2(c_2 + W(f(c_1 + W))) \frac{\partial(c_1 + W(h_1(c_1 + W)))}{\partial W} && \text{using chain rule} \\ &= h'_2(c_2 + W(f(c_1 + W))) (h_1(c_1 + W) + Wh'_1(c_1 + W)) && \text{using product rule} \\ &= h'_2(c_2 + W(f(c_1 + W)))h_1(c_1 + W) + h'_2(c_2 + W(h(c_1 + W)))Wh'_1(c_1 + W) \\ &= \frac{\partial h_2}{\partial z_2} \frac{\partial z_2}{\partial W} + \frac{\partial h_2}{\partial z_2} \frac{\partial z_2}{\partial h_1} \frac{\partial h_1}{\partial W} = \frac{\partial h_2}{\partial W} + \frac{\partial h_2}{\partial h_1} \frac{\partial h_1}{\partial W} \end{aligned}$$

Gradient Vanishing and/or Explosion

$$\frac{\partial \mathcal{C}_t}{\partial W} = \sum_{k=0}^t \frac{\partial \mathcal{C}_t}{\partial \hat{y}_t} \frac{\partial \hat{y}_t}{\partial h_t} \left(\prod_{j=k+1}^t \frac{\partial h_j}{\partial h_{j-1}} \right) \frac{\partial h_k}{\partial z_k} \frac{\partial z_k}{\partial W}$$

before

$$h_t = \tanh(Ux_t + Wh_{t-1})$$

$$\hat{y}_t = \text{softmax}(Vh_t)$$

hard to analyse $\frac{\partial h_t}{\partial h_k}$

alternative

$$h_t = Ux_t + Wf(h_{t-1})$$

$$\hat{y}_t = Vf(h_t)$$

easier to analyse $\frac{\partial h_t}{\partial h_k}$

In alternative representation:

$$\frac{\partial h_t}{\partial h_k} = \prod_{j=k+1}^t \frac{\partial h_j}{\partial h_{j-1}} = \prod_{j=k+1}^t W \times \text{diag}[f'(h_{j-1})]$$

This is because:

$$\begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} W_{1,1} & W_{1,2} \\ W_{2,1} & W_{2,2} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} w_{1,1}x_1 + w_{1,2}x_2 \\ w_{2,1}x_1 + w_{2,2}x_2 \end{bmatrix} \Rightarrow \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_1}{\partial x_2} \\ \frac{\partial y_2}{\partial x_1} & \frac{\partial y_2}{\partial x_2} \end{bmatrix} = W$$

Gradient vanishing and/or exploding: Matrix norm

Define matrix norm from vector norm:

$$\|A\| = \sup \{ \underbrace{\|Ax\|}_{\text{vector norm}} : x \in \mathbb{R}^n \text{ with } \underbrace{\|x\|}_{\text{vector norm}} = 1 \}$$

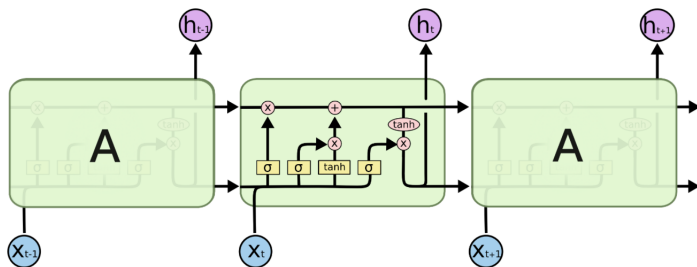
$$\begin{aligned} \left\| \frac{\partial h_j}{\partial h_{j-1}} \right\| &\leq \beta_W \beta_s \\ \left\| \frac{\partial h_t}{\partial h_k} \right\| &= \left\| \prod_{j=k+1}^t \frac{\partial h_j}{\partial h_{j-1}} \right\| = \left\| \prod_{j=k+1}^t W \times \text{diag}[f'(h_{j-1})] \right\| \leq (\beta_W \beta_s)^{t-k} \end{aligned}$$

Possible solution:

- ▶ Let $f(x) = \max(0, x)$, i.e., another activation function, for example, ReLU helps with gradient.
- ▶ Initialise W to be the identity matrix.

Long Short Term Memory (LSTM)

Looking at very complicated structure. But it works!

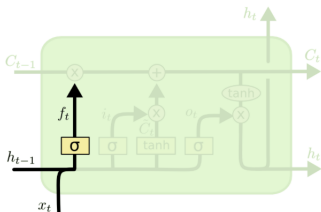


- ▶ There is a concept of Cell State $\{C_t\}$ in addition to state $\{h_t\}$.
- ▶ <http://colah.github.io/posts/2015-08-Understanding-LSTMs/>

Long Short Term Memory (LSTM): forget and input gate

forget gate:

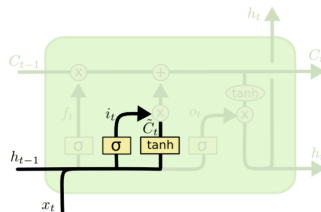
$$f_t = \sigma(W_f[h_{t-1}, x_t] + b_f)$$



input gate:

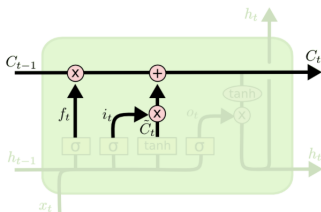
$$i_t = \sigma(W_i[h_{t-1}, x_t] + b_i)$$

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



state update:

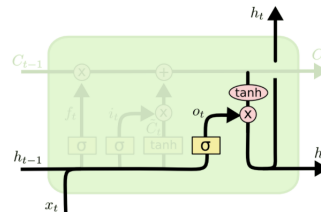
$$C_t = f_t \odot C_{t-1} + i_t \odot \tilde{C}_t$$



output gate:

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

$$h_t = o_t \odot \tanh(C_t)$$



- ▶ a compact form of representation:

$$\begin{bmatrix} i \\ f \\ o \\ \tilde{C} \end{bmatrix} = \begin{bmatrix} \sigma \\ \sigma \\ \sigma \\ \tanh \end{bmatrix} W \begin{bmatrix} h_{t-1} \\ x_t \end{bmatrix} \quad C_t = f_t \odot C_{t-1} + i \odot \tilde{C}_t$$

$$h_t = o_t \odot \tanh(C_t)$$

- ▶ in vanilla RNN, multiple by the same \mathbf{W} , in LSTM, f_t changes each time step
- ▶ element-wise multiplication (LSTM) is nicer than full matrix multiplication RNN
- ▶ in LSTMs, cell state C_t . The derivative of consecutive States is of the form:

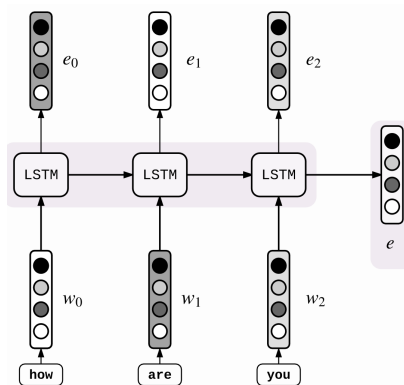
$$\begin{aligned} C_t &= f_t \times C_{t-1} + i_t \times \tilde{C}_t \\ &= f_t \times C_{t-1} + i_t \times \tanh(W_C[h_{t-1}, x_t] + b_C) \\ &= f_t(C_{t-1})C_{t-1} + i_t \underbrace{(h_{t-1}(C_{t-1})) \times \tanh(W_C[o_{t-1}(h_{t-1}(C_{t-1})) \times \tanh(C_{t-1}), x_t] + b_C)}_{\xi(C_{t-1})} \end{aligned}$$

$$\frac{\partial C_t}{\partial C_{t-1}} = \underbrace{f_t}_{\text{gradient-super highway}} + \underbrace{\frac{\partial f_t}{\partial C_{t-1}} C_{t-1} + \frac{\partial \xi(C_{t-1})}{\partial C_{t-1}} C_{t-1}}_{\text{contains exponentially fast decay function}}$$

- ▶ of course, f_t may still close to zero
- ▶ **trick is to** initialize bias to positive, e.g., $f_t = \sigma(W_f[h_{t-1}, x_t] + \text{+ve})$ so to make f_t closer to 1 initially

Vanilla Seq2Seq: encoder

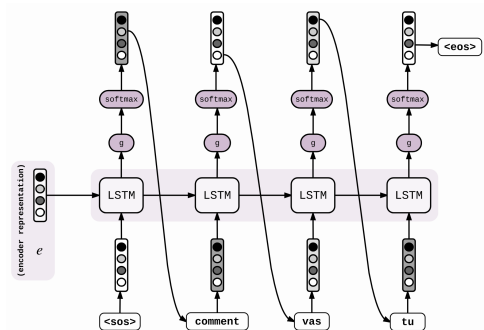
- ▶ Sutskever et., al, 2014, *Sequence to sequence learning with neural networks*
- ▶ at encoder: last neural representation e “**summarizes**” entire encoder sentence
- ▶ this neural representation is to be used at the decoder
- ▶ it uses RNN(LSTM) each time t



<https://guillaumegenthiel.github.io/sequence-to-sequence.html>

Vanilla Seq2Seq: decoder

- ▶ Sutskever et., al, 2014, *Sequence to sequence learning with neural networks*
- ▶ at decoder: it uses last neural representation e from encoder
- ▶ it generates one word at the time
- ▶ during **training**, decoder sentence to minimize the cross entropy error



<https://guillaumequenthal.github.io/sequence-to-sequence.html>

Seq2Seq: beam-search (1)

- in theory, decoder generates words **jointly**, so how we may compute:

$$\{\hat{y}_1, \dots, \hat{y}_T\} = \arg \max_{y_1, \dots, y_T} \left[\Pr(y_1, \dots, y_T | \mathbf{x}) \equiv \Pr(y_1 | \mathbf{x}) \Pr(y_2 | y_1, \mathbf{x}), \dots, \Pr(y_T | y_1, \dots, y_{T-1}, \mathbf{x}) \right]$$

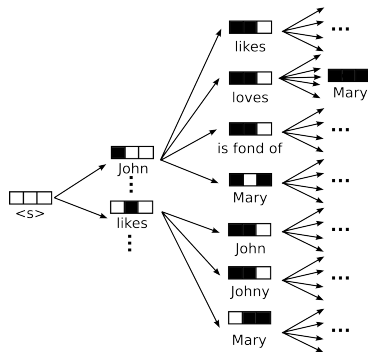
- select all:** **tree-width** = N , so we get answer to be:

$$\{\hat{y}_1, \dots, \hat{y}_T\} = \arg \max_{y_1, \dots, y_T} \left[\Pr(y_1 | \mathbf{x}) \Pr(y_2 | y_1, \mathbf{x}) \Pr(y_3 | y_1, y_2, \mathbf{x}) \dots, \Pr(y_T | y_1, \dots, y_{T-1}, \mathbf{x}) \right]$$

in each depth, keep (**select**) **full width** N , until its full depth T , before select a best path

(**accurate, but computationally infeasible**): N^T paths!

- select one:** **tree-width** = 1 , **greedy algorithm** (def. making locally optimal choice at each stage, to "approximately" a global optimum)
select best word at each depth t : choose one branch in a depth, and discard rest of sibling branches
(**fast & storage efficient, but accuracy-wise bad**)



$$\{\hat{y}_1, \dots, \hat{y}_T\} \approx \{\tilde{y}_1, \dots, \tilde{y}_T\}$$

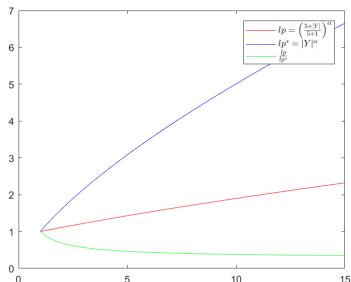
$$= \left\{ \tilde{y}_1 \equiv \arg \max_{y_1} \Pr(y_1 | \mathbf{x}), \tilde{y}_2 \equiv \arg \max_{y_2} \Pr(y_2 | \tilde{y}_1, \mathbf{x}), \dots, \tilde{y}_T \equiv \arg \max_{y_T} \Pr(y_T | \tilde{y}_1, \dots, \tilde{y}_{T-1}, \mathbf{x}) \right\}$$

- ▶ tree width of N and 1 are both **not ideal**, so we go for a compromise
- ▶ easy, select tree width of $1 < W < N$:
- ▶ loop from 1 to T , at each depth t :
 1. use W **most probable** branches chosen at the previous depth
 2. extend each W branch by depth $+1$, and to generate $W \times N$ candidate branches
 3. choose the W **most probable** branches, and go for next iteration

beam-search: more sophisticated normalization (1)

- ▶ Wu et. al., (2016), "Google's Neural Machine Translation System: Bridging the Gap"
- ▶ to **maximize** scores generated by the model:

$$s(Y, X) = \frac{1}{\text{lp}(Y)} \log P(Y|X) + \text{cp}(X, Y)$$



- ▶ instead of normalize by the length $lp^* = |Y|^\alpha$, it uses a different normalization $lp(Y)$:

$$lp(Y) = \frac{(5 + |Y|)^\alpha}{(5 + 1)^\alpha}$$

- ▶ $lp(Y)$ penalizes as much as $lp^*(Y)$ when $|Y|$ is small, then it "gently" drops as $|Y|$ increases

beam-search: more sophisticated normalization (2)

$$s(Y, X) = \frac{1}{\text{lp}(Y)} \log P(Y|X) + \text{cp}(X, Y)$$

- ▶ it needs also to maximize **coverage penalty**:

$$\text{cp}(X, Y) = \beta \sum_{j=1}^{|X|} \log \left(\min \left(\sum_{i=1}^{|Y|} a_{i,j}, 1.0 \right) \right)$$

where $a_{i,j}$ is attention probability of i -th target **decoder** word on j -th source **encoder** word

- ▶ we know that:

$$\sum_{j=1}^{|X|} a_{i,j} = 1 \quad \text{and} \quad \sum_{i=1}^{|Y|} a_{i,j} \neq 1 \text{ in general}$$

- ▶ think \mathbf{a} as a matrix of size $|Y| \times |X|$, which we distribute a total mass of $|Y|$ in value among all of its elements, for example, $|X| = |Y| = 3$:

$$\mathbf{a} = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}$$

minimized $\text{cp}(X, Y)$

$$\mathbf{a} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

maximized $\text{cp}(X, Y)$

- ▶ favor translations that fully cover source sentence according to the attention module
- ▶ lastly, one may encourage the decoder to be longer than the encoder:
`opennmt.net/OpenNMT/translation/beam_search/`

$$\text{ep}(X, Y) = \gamma \frac{|Y|}{|X|}$$

Sequence to Sequence with Attention

- ▶ **encoders** have hidden states, $\{z_1, \dots, z_m\} \in \mathbb{R}^h$
- ▶ **decoders** have hidden states, $\{h_1, \dots, h_n\} \in \mathbb{R}^h$
- ▶ compute **dot-product**: $e_{i,j} = h_i^\top z_j$
- ▶ **attentions** between i^{th} decoder state and j^{th} encoder state is:

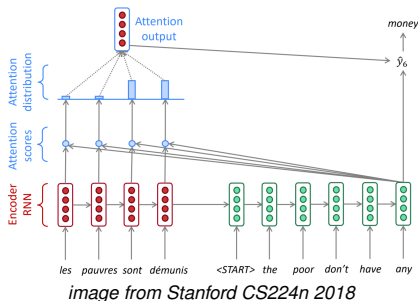
$$a_{ij} = \frac{\exp(e_{i,j})}{\sum_{t=1}^m \exp(e_{i,t})} = \frac{\exp(h_i^\top z_j)}{\sum_{t=1}^m \exp(h_i^\top z_t)}$$

- ▶ each i^{th} decoder has $\mathbf{a}_i = \{a_{i,1}, \dots, a_{i,m}\}$ attention weights of the encoder
- ▶ **condition vector** c_i for each decode word i :

$$c_i = \sum_{j=1}^m a_{i,j}(z_j)$$

- ▶ new **augmented decoder state** \tilde{h}_t :

$$\tilde{h}_t = [c_i; h_t] \in \mathbb{R}^{2h}$$



something about **dot-product**: $e_{i,j} = h_i^\top z_j$, many version exist:

1. $e_{i,j} = h_i^\top \mathbf{W} z_j$
enable h and z have different dimensionality
2. $e_{i,j} = v_i^\top \tanh(\mathbf{W}_1 h_i + \mathbf{W}_2 z_j)$
(v_i , \mathbf{W}_1 , \mathbf{W}_2) are parameters of this dot-product
Pointer Networks uses this!

Sequence to Sequence with Attention: issues (1)

- ▶ **issue one:** decoder sometimes repeat themselves (e.g. "machine learning machine learning ...")
solution (See, et., al, 2017), *Get To The Point: Summarization with Pointer-Generator Networks*

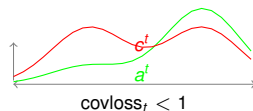
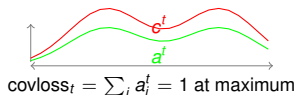
- ▶ **coverage vector** Sum of attention distributions so far:

$$c^t = \sum_{t'=0}^{t-1} a^{t'}$$

- ▶ penalize overlap between **coverage vector** c^t and new attention distribution a^t :

$$\text{covloss}_t = \sum_i \min(a_i^t, c_i^t)$$

- ▶ the above equation can be understood as follows:
imagine $c_i^t \geq a_i^t \forall i$, then $\text{covloss}_t = 1$, which is its **maximum**, this happens when covloss_t is a multiplicative envelop of a^t :



- ▶ in essence, covloss_t tries to make a^t distributed differently to c^t

Sequence to Sequence with Attention: issues (2)

- ▶ **issue two** decoder may not be able to translate “out-of-vocabulary words” such as names of a company
- ▶ suppose to have the following text summarization task:
 - ▶ **original text:**
“The QueenslandCo has made all reasonable efforts to ensure that this material has been reproduced with the consent of NSWCo”
 - ▶ **summarized text:**
“NSWCo allowed QueenslandCo to reuse its content”
 - ▶ some of the words should appear **as is**
- ▶ RNN-based summarization may replace “Mary” with “Jane” and “Sydney” with “Melbourne” since these word embeddings tend to cluster (and hence their dot product are similar!)
- ▶ **solution** “Pointer Networks” may be handy to come to help!

What is Pointer Networks anyway?

- ▶ (Vinyals, 2016), *Pointer Networks*
- ▶ “Seq2Seq with attention” is to predict **content** of next word
- ▶ “Pointer Networks” is to predict next **position** of encoding sequence
- ▶ $e_{i,j} = v_i^\top \tanh(\mathbf{W}_1 h_i + \mathbf{W}_2 z_j)$

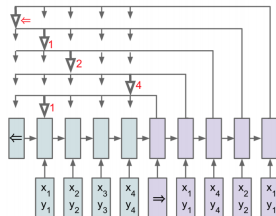
$$a_{ij} = \frac{\exp(e_{i,j})}{\sum_{t=1}^m \exp(e_{i,t})} = \frac{\exp(h_i^\top z_j)}{\sum_{t=1}^m \exp(h_i^\top z_t)}$$

- ▶ instead of compute **conditional vector** c_i and concatenate with h_i as the case of “Seq2Seq with attention”, it performs:

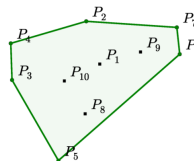
$$\Pr(C_i | C_1, \dots, C_{i-1}, \mathcal{P}) = \text{softmax}(e_{i,1}, \dots, e_{i,n})$$

- ▶ now that we apply Pointer Network to “copy” rare words from encoder to decoder, what about generating words that don't appear in the encoder?
- ▶ the answer is a **mixture model** that does both **copy (extraction)** and **generation (abstraction)**

- ▶ pointer network structure:

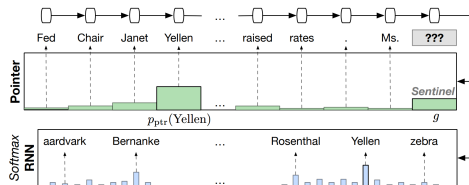


- ▶ it could solve combinatorial geometry problems:



Pointer Sentinel Mixture Models (1)

- (Merity, 2016), *Pointer sentinel mixture models*
- combines **abstraction** and **extraction** together



$$p(\text{"Yellen"}) = g \times p_{\text{vocab}}(\text{"Yellen"}) + (1 - g) \times p_{\text{ptr}}(\text{"Yellen"})$$

- g is mixture gate, uses sentinel to dictate how much probability mass to give to vocabulary
- note that PSMM paper doesn't discuss seq2seq, instead it is about generate $\Pr(y_N | w_1, \dots, w_{N-1})$

Pointer Sentinel Mixture Models (2): its design

- ▶ simplest way to compute an attention score with all past hidden states $\{h\}_i = 1^{N-1}$, with each hidden state $h_i \in \mathbb{R}^H$
- ▶ However, when computing score for most recent word with hidden state h_N , if it's a **repeating word** with previous hidden state h_{N-1} , then $h_N^\top h_{N-1} = \|h_N\|_{L_2}^2$, i.e., big, and hence it is more likely to generate itself again!
- ▶ the paper hence project the previous hidden state h_{N-1} to a query vector q :

$$q = \tanh(Wh_{N-1} + b)$$

- ▶ so, that dot-product between “candidate state” and “previous state” pair is no longer $e_{N,N-1} = h_N^\top h_{N-1}$, instead it's $e_{N,N-1} = h_N^\top q$
- ▶ rest is standard: $a = \text{softmax}(e)$

Beyond Seq2Seq with Attention using LSTM!

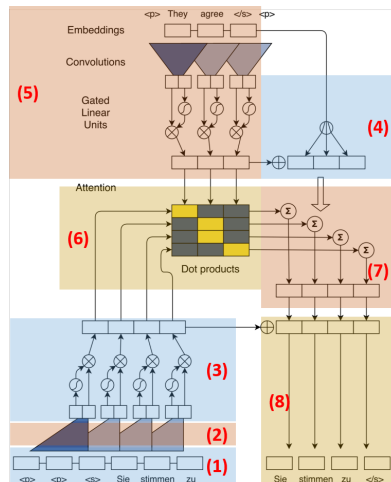
- ▶ Sequence-to-sequence (Seq2Seq) using LSTM building block has been **the method** since 2015!
- ▶ however, LSTM cannot be parallelized, so what then? two replacement methods stood out in second half of 2017:
- ▶ “attention is all you need” (Google Research)
- ▶ “Convolution Sequence to Sequence” (Facebook AI Research)

Convolution Sequence to Sequence (1): Decoder

- ▶ (Gehring, 2017), *Convolutional sequence to sequence learning*
- ▶ (1) these are decoder raw inputs $\{g_i \equiv h_i^{(0)}\}$ representing input sentence $\{x_1, \dots, x_n\}$
- ▶ (2) concatenate features within window size k :
 1. for each decoder position i , take a k element set $\{g_i \equiv h_i^{(0)}\}$: $\{h_{(i-k)/2}^{(0)}, \dots, h_{(i+k)/2}^{(0)}\}$
 2. concatenate to form a vector $\hat{h}_i^{(0)}$, which has size $k \times d$
- ▶ (3) repeat the above two steps for several layers, relationship between current l and previous $l-1$ layers are:

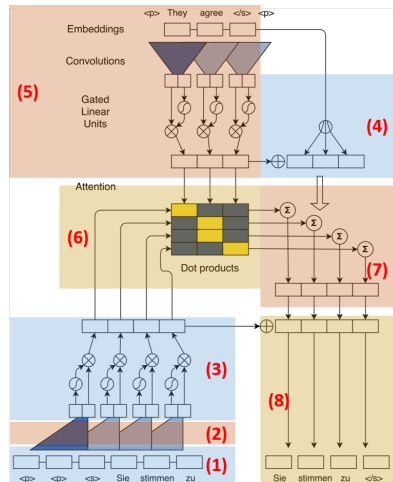
$$h_i^{(l)} = v(W^l \hat{h}_i^{(l-1)}) \quad \text{where } v(\cdot) \text{ is **gated convolution**}$$

- ▶ during **training**, each **decoding word** g_i can be embedded to $h_i^{(l)}$ in parallel



Convolution Sequence to Sequence (2): Encoder

- ▶ (4) for **encoder** produce sequence $\{e_1, \dots, e_m\}$ where $e_j = w_j + p_j$: word embedding + position embedding
- ▶ (5) the process to embed encoder sequence into the last layer: $\{z_1^u, \dots, z_m^u\}$ using same process as decoder



Convolution Sequence to Sequence (3): Put together

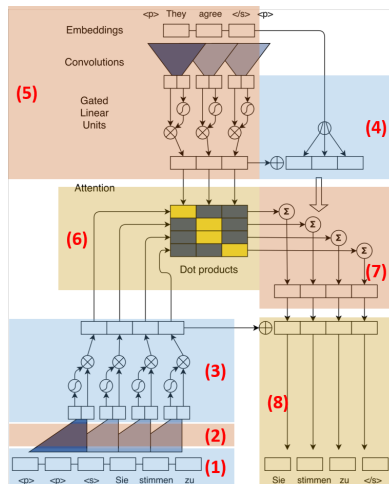
- (6) to compute attention $a_{ij}^{(l)}$:

$$d_i^{(l)} = W_d^{(l)} h_i^{(l)} + b_d^{(l)} + g_i \quad a_{ij}^{(l)} = \frac{\exp(d_i^{(l)\top} z_j^{(u)})}{\sum_{t=1}^m \exp(d_i^{(l)\top} z_t^{(u)})}$$

- note that this is slightly different to the diagram: the paper has only dot product term ($d_i^{(l)} \odot z_j^{(u)}$)
- (7) to compute condition vector c_i^l for each decoding word i :

$$c_i^{(l)} = \sum_{j=1}^m a_{ij}^{(l)} (z_j^{(u)} + e_j)$$

- (8) to generate the sequence using predict y_{i+1} from $\{c_i^l + h_i^l\}_{l=1}^L$
- during testing:
 - y_i is generated one at the time
 - the “dot product” table in (6) is increase one row at the time



Gated Convolutional Network

- ▶ so what is **gated convolution** used in convolutional seq2seq?
- ▶ Yann N. Dauphin, *Language Modeling with Gated Convolutional Networks*
- ▶ look at last box **gating**, reduce vanishing gradient problem:

1. gradient of LSTM-style gating:

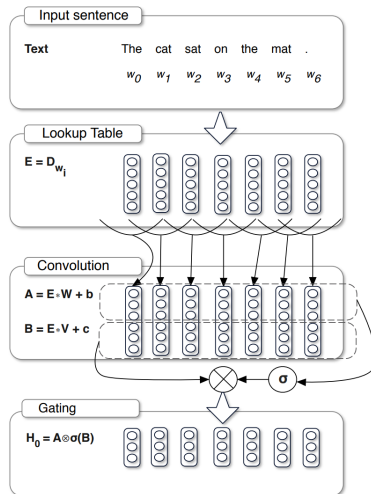
$$\begin{aligned} h_t &= o_t \odot \tanh(C_t) \\ &= \sigma(W_o[h_{t-1}, x_t] + b_o) \odot \tanh(C_t) \end{aligned}$$

writing it more generically:

$$\begin{aligned} \nabla[\tanh(X) \odot \sigma(X)] \\ = \underbrace{\tanh'(X)}_{\text{down scaling}} \nabla X \odot \sigma(X) + \underbrace{\sigma'(X)}_{\text{down scaling}} \nabla(X) \odot \tanh(X) \end{aligned}$$

2. Gated Convolution Networks

$$\begin{aligned} \nabla[X \odot \sigma(X)] \\ = \underbrace{\nabla X \odot \sigma(X)}_{\text{no down scaling path}} + \underbrace{\sigma'(X)}_{\text{down scaling}} \nabla(X) \odot X \end{aligned}$$



Transformer Networks: Dot-Product Attention

- ▶ let (q, K, V) be tuples: the Dot-Product Attention (DPA) is defined as:

$$A(q, K, V) = \sum_i \frac{\exp[q^\top k_i]}{\underbrace{\sum_j \exp[q^\top k_j]}_{a_i}} v_i$$

- ▶ in the case of **seq2seq** with attention:

► $q = h$

- ▶ $k_i = v_i = z_i$

- ▶ $A(q, K, V) = A(h_j, z, z) = c_i$, where is our **conditional** or **context** vector:

$$a_{ij} = \frac{\exp(e_{i,j})}{\sum_{t=1}^m \exp(e_{i,t})} = \frac{\exp(h_i^\top z_j)}{\sum_{t=1}^m \exp(h_i^\top z_t)}$$

- now we have many $Q = \{q_i\}$, e.g., N words in the decoder, we can rewrite it as:

$$A(Q, K, V) = \text{softmax}(QK^T)V$$

$$\underbrace{\left[\begin{array}{ccc} - & q & - \\ & d_k & \end{array} \right]}_{A(q,K,V)} \left[\begin{array}{c} | \\ \vdots \\ k_1 \\ \vdots \\ k_m \\ \vdots \\ | \end{array} \right] \left\{ \begin{array}{c} \vdots \\ \vdots \\ \vdots \\ \vdots \end{array} \right\} d_k \left[\begin{array}{ccc} - & & \\ \vdots & v_1 & \vdots \\ - & v_m & - \end{array} \right] \Rightarrow \underbrace{\left[\begin{array}{ccc} - & & \\ \vdots & q_1 & \vdots \\ - & q_n & - \end{array} \right]}_{A(Q,K,V)} \left[\begin{array}{c} | \\ \vdots \\ k_1 \\ \vdots \\ k_m \\ \vdots \\ | \end{array} \right] \left\{ \begin{array}{c} \vdots \\ \vdots \\ \vdots \\ \vdots \end{array} \right\} d_k \left[\begin{array}{ccc} - & & \\ \vdots & v_1 & \vdots \\ - & v_m & - \end{array} \right]$$

Transformer Networks: Scaled Dot-Product Attention

Vaswani, et. al, (2017), "Attention Is All You Need" (Google)

problem:

- ▶ as d_k is larger variance of $q^\top k$ increases:
- ▶ as a result, some dot product values gets very large, with $\exp(\cdot)$, softmax \mathbf{p} gets peaky!
- ▶ remember derivative of cross-entropy between softmax \mathbf{p} and \mathbf{y} is:

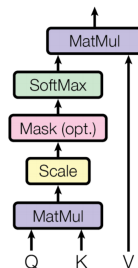
$$C(\mathbf{z}) = - \sum_{k=1}^K y_k [\log(p_k)] = - \sum_{k=1}^K y_k \left[\log \left(\frac{\exp^{z_k}}{\sum_i \exp^{z_i}} \right) \right]$$
$$\Rightarrow \frac{C(\mathbf{z})}{\partial \mathbf{z}} = (\mathbf{p} - \mathbf{y})$$

- ▶ with a peaky softmax, lots of element in gradient vector $\frac{C(\mathbf{z})}{\partial \mathbf{z}}$ are zero!

solution:

- ▶ scale by length of d_k :

$$A(Q, K, V) = \text{softmax} \left(\frac{QK^\top}{\sqrt{d_k}} \right) V$$



- ▶ "mask (opt.)" is only used at decoder during training

Self-attention and Multi-head attention

- ▶ **generic** input vectors could be (Q, K, V)
- ▶ when allow some equal signs, for example, $Q = K = V$, it achieves **self-attention**!
- ▶ **even better** can we let words to have multiple ways of interactions with each other?
- ▶ **Multi-head attention**!

1. **loop** through $i \in \{1 \dots h\}$, for each i -th iteration:

- ▶ linear transform Q, K, V into several lower dimensional spaces, to obtain

$$\text{head}_i = (QW_i^q, KW_i^k, VW_i^v)$$

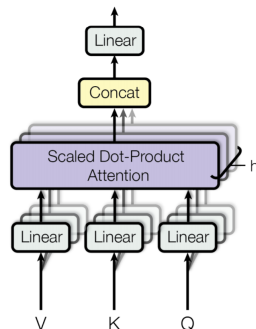
- ▶ each iteration i correspond to **one "surface"** of the ["linear", "Scaled Dot-Product Attention"] on the diagram

2. then concatenate to produce output matrix **H**

$$\mathbf{H} = [\text{head}_1, \dots, \text{head}_h]$$

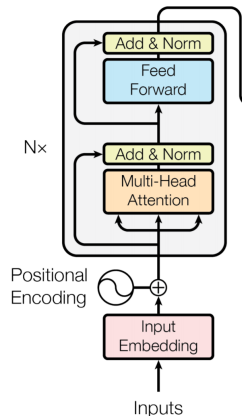
3. finally,

$$\text{MultiHead}(Q, K, V) = \mathbf{H}\mathbf{W}^o$$



Attention is all you need: encoder

- ▶ for **encoder** each block, use same ($Q = K = V$) from previous layer
- ▶ all the goodies: ReLU + ResNet+ NN + LayerNorm
- ▶ blocks repeated $N \times$ times
- ▶ unlike RNN, using attention loose the ordering of the words in encoder, therefore, **explicit position encoding** is required



Attention is all you need: decoder

- ▶ again, all the goodies: ReLU + ResNet+ NN + LayerNorm
- ▶ during training: masked decoder self-attention on previously generated outputs
- ▶ Encoder-Decoder Attention: Q come from previous decoder layer and K and V come from output of encoder
- ▶ the above is similar to **seq2seq with attention** $Q = h$ from decoder, $K = V = z$ from encoder
- ▶ blocks repeated N times

