Reinforced Self-Attention Network:
a Hybrid of Hard and Soft Attention for Sequence Modeling

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Abstract

Many natural language processing tasks solely rely on sparse dependencies between a few tokens in a sentence. Soft attention mechanisms show promising performance in modeling local/global dependencies by soft probabilities between every two tokens, but they are not effective and efficient when applied to long sentences. By contrast, hard attention mechanisms directly select a subset of tokens but are difficult and inefficient to train due to their combinatorial nature. In this paper, we integrate both soft and hard attention into one context fusion model, "reinforced self-attention (ReSA)", for the mutual benefit of each other. In ReSA, a hard attention trims a sequence for a soft self-attention to process, while the soft attention feeds reward signals back to facilitate the training of the hard one. For this purpose, we develop a novel hard attention called "reinforced sequence sampling (RSS)", selecting tokens in parallel and trained via policy gradient. Using two RSS modules, ReSA efficiently extracts the sparse dependencies between each pair of selected tokens. We finally propose an RNN/CNN-free sentence-encoding model, "reinforced self-attention network (ReSAN)", solely based on ReSA. It achieves state-of-the-art performance on both Stanford Natural Language Inference (SNLI) and Sentences Involving Compositional Knowledge (SICK) datasets.

1 Introduction

Equipping deep neural networks (DNN) with attention mechanisms provides an effective and parallelizable approach for context fusion and sequence compression. It achieves compelling time efficiency and state-of-the-art performance in a broad range of natural language processing (NLP) tasks, such as neural machine translation [Bahdanau *et al.*, 2015; Luong *et al.*, 2015], dialogue generation [Shang *et al.*, 2015], machine reading/comprehension [Seo *et al.*, 2017], natural language inference [Liu *et al.*, 2016], etc. Recently, some neural networks based solely on attention, especially self-attention, outperform traditional recurrent or convolutional neural networks on NLP tasks, such as machine translation

[Vaswani *et al.*, 2017] and sentence embedding [Shen *et al.*, 2017a], which further demonstrates the power of attention mechanisms in capturing contextual dependencies.

Soft and hard attention are the two main types of attention mechanisms. In soft attention [Bahdanau *et al.*, 2015], a categorical distribution is calculated over a sequence of elements. The resulting probabilities reflect the importance of each element and are used as weights to produce a context-aware encoding that is the weighted sum of all elements. Hence, soft attention only requires a small number of parameters and less computation time. Moreover, soft attention mechanism is fully differentiable and thus can be easily trained by end-to-end back-propagation when attached to any existing neural net. However, the softmax function usually assigns small but non-zero probabilities to trivial elements, which will weaken the attention given to the few truly significant elements.

Unlike the widely-studied soft attention, in hard attention [Xu *et al.*, 2015], a subset of elements is selected from an input sequence. Hard attention mechanism forces a model to concentrate solely on the important elements, entirely discarding the others. In fact, various NLP tasks solely rely on very sparse tokens from a long text input. Hard attention is well suited to these tasks, because it overcomes the weaknesses associated with soft attention in long sequences. However, hard attention mechanism is time-inefficient with sequential sampling and non-differentiable by virtue of their combinatorial nature. Thus, it cannot be optimized through back-propagation and more typically rely on policy gradient, e.g., REINFORCE [Williams, 1992]. As a result, training a hard attention model is usually an inefficient process – some even find convergence difficult – and combining them with other neural nets in an end-to-end manner is problematic.

However, soft and hard attention mechanisms might be integrated into a single model to benefit each other in overcoming their inherent disadvantages, and this notion motivates our study. Specifically, a hard attention mechanism is used to encode rich structural information about the contextual dependencies and trims a long sequence into a much shorter one for a soft attention mechanism to process. Conversely, the soft one is used to provide a stable environment and strong reward signals to help in training the hard one. Such method would improve both the prediction quality of the soft attention mechanism and the trainability of the hard attention mechanism, while boosting the ability to model contextual depen-

dencies. To the best of our knowledge, the idea of combining hard and soft attention within a model has not yet been studied. Existing works focus on only one of the two types.

In this paper, we first propose a novel hard attention mechanism called "reinforced sequence sampling (RSS)", which selects tokens from an input sequence in parallel, and differs from existing ones in that it is highly parallelizable without any recurrent structure. We then develop a model, "reinforced self-attention (ReSA)", which naturally combines the RSS with a soft self-attention. In ReSA, two parameter-untied RSS are respectively applied to two copies of the input sequence, where the tokens from one and another are called dependent and head tokens, respectively. ReSA only models the sparse dependencies between the head and dependent tokens selected by the two RSS modules. Finally, we build an sentence-encoding model, "reinforced self-attention network (ReSAN)", based on ReSA without any CNN/RNN structure.

We experimentally test ReSAN on natural language inference and semantic relatedness tasks. The results show that ReSAN achieves the best test accuracy among all sentence-encoding models on the official leaderboard of the Stanford Natural Language Inference (SNLI) dataset, and state-of-the-art performance on the Sentences Involving Compositional Knowledge (SICK) dataset. Compared to the commonly-used models, ReSAN is more efficient and has better prediction quality than existing recurrent/convolutional neural networks, self-attention networks, and even well-designed models (e.g., semantic tree or external memory based models).

Notation: 1) lowercase denotes a vector; 2) bold lowercase denotes a sequence of vectors (stored as a matrix); and 3) uppercase denotes a matrix or a tensor.

We provide extensive material in appendix, which includes **further model comparison**, **a full background of soft-attention**, etc.

2 Background

2.1 Attention

Given an input sequence $\boldsymbol{x} = [x_1, \ldots, x_n] \in \mathbb{R}^{d_e \times n}$ ($x_i \in \mathbb{R}^{d_e}$ denotes the embedded vector of i-th element), and the vector representation of a query q, an vanilla *attention* mechanism uses a parameterized compatibility function $f(x_i, q)$ to computes an alignment score between q and each token x_i as the attention of q to x_i [Bahdanau *et al.*, 2015]. A softmax function is then applied to the alignment scores $a \in \mathbb{R}^n$ over all tokens to generate a categorical distribution $p(v|\boldsymbol{x}, q)$, where $v = i$ implies that token x_i is selected according to its relevance to query q. This can be formally written as

$$a = [f(x_i, q)]_{i=1}^n, \quad (1)$$
$$p(v|\boldsymbol{x}, q) = \text{softmax}(a). \quad (2)$$

The output of attention, s, is the expectation of sampling a token according to the categorical distribution $p(v|\boldsymbol{x}, q)$, i.e.,

$$s = \sum_{i=1}^n p(v = i|\boldsymbol{x}, q)x_i = \mathbb{E}_{i \sim p(v|\boldsymbol{x}, q)}[x_i]. \quad (3)$$

Multi-dimensional (multi-dim) attention mechanism [Shen *et al.*, 2017a] extends the vanilla one [Bahdanau *et al.*, 2015]

to a feature-wise level, i.e., each feature of every token has an alignment score. Hence, rather than a scalar, the output of $f(x_i, q)$ is a vector with the same dimensions as the input, and the resulting alignment scores compose a matrix $a \in \mathbb{R}^{d_e \times n}$. Such feature-level attention has been verified in terms of its ability to capture the subtle variances of different contexts.

2.2 Self-Attention

Self-attention is a special case of attention where the query q stems from the input sequence itself. Hence, self-attention mechanism can model the dependencies between tokens from the same sequence. Recently, a variety of self-attention mechanisms have been developed, each serving a distinct purpose, but most can be roughly categorized into two types, token2token self-attention and source2token self-attention.

token2token self-attention mechanisms aim to produce a context-aware representation for each token in light of its dependencies on other tokens in the same sequence. The query q is replaced with the token x_j, and the dependency of x_j on another token x_i is computed by $f(x_i, x_j)$. There are two proposed self-attentions in this type, i.e., scaled dot-product attention which composes the multi-head attention [Vaswani *et al.*, 2017] and masked self-attention which leads to directional self-attention [Shen *et al.*, 2017a]. Because the latter experimentally outperforms the former, we select the masked self-attention as our fundamental soft self-attention module.

Masked Self-Attention is more sophisticated than scaled dot-product attention in that, it uses multi-dim and multi-layer perceptron with an additional position mask, rather than a scaled dot-product, as the compatibility function, i.e.,

$$f(x_i, x_j) =$$
$$c \cdot \tanh\left([W^{(1)}x_i + W^{(2)}x_j + b^{(1)}]/c\right) + M_{ij}, \quad (4)$$

where c is a scalar and M is the mask with each entry $M_{ij} \in \{-\infty, 0\}$. When $M_{ij} = -\infty$, applying the softmax function to a results in a zero probability, $p(z = i|\boldsymbol{x}, x_j) = 0$, which switches off the attention of x_j to x_i. An asymmetric mask where $M_{ij} \neq M_{ji}$ enforces directional attention between x_i and x_j, which can encode temporal order information. Two positional masks have been designed to encode the forward and backward temporal order, respectively, i.e.,

$$M_{ij}^{fw} = \begin{cases} 0, & i < j \\ -\infty, & \text{otherwise} \end{cases} \qquad M_{ij}^{bw} = \begin{cases} 0, & i > j \\ -\infty, & \text{otherwise} \end{cases}$$

In forward and backward masks, $M_{ii} = -\infty$. Thus, the attention of a token to itself is blocked, so the output of masked self-attention mechanism comprises the features of the context around each token rather than context-aware features.

Directional self-attention uses a fusion gate to combine the embedding of each token with its context. Specifically, a fusion gate combines the input and output of a masked self-attention to produce context-aware representations. This idea is similar to the highway network [Srivastava *et al.*, 2015].

source2token self-attention mechanisms [Shen *et al.*, 2017a] remove the query q from the compatibility function in Eq.(1) and directly compresses a sequence into a vector representation calculated from the dependency between each token x_i and the entire input sequence $\boldsymbol{x}$. Hence, this form of self-attention is highly data- and task- driven.

3 Proposed Models

This section begins by introducing a hard attention mechanism called RSS in Section 3.1, followed by integrating the RSS with a soft self-attention mechanism into a context fusion model called ReSA in Section 3.2. Finally, a model named ReSAN, based on ReSA, is designed for sentence encoding tasks in Section 3.3

3.1 Reinforced Sequence Sampling (RSS)

The goal of hard attention mechanism is to select a subset of critical tokens that provides sufficient information to complete downstream tasks, so any further computations on the trivial tokens can be saved. In the following, we introduce a hard attention mechanism called RSS. Given an input sequence $\boldsymbol{x} = [x_1, \ldots, x_n]$, RSS generates an equal-length sequence of binary random variables $\boldsymbol{z} = [z_1, \ldots, z_n]$ where $z_i = 1$ implies that x_i is selected whereas $z_i = 0$ indicates that x_i is discarded. In RSS, the elements of $\boldsymbol{z}$ are sampled in parallel according to probabilities computed by a learned attention mechanism. This is more efficient than using MCMC with iterative sampling. The particular aim of RSS is to learn the following product distribution.

$$p(\boldsymbol{z}|\boldsymbol{x}; \theta_r) = \prod_{i=1}^{n} p(z_i|\boldsymbol{x}; \theta_r), \qquad (5)$$

$$\text{where } p(z_i|\boldsymbol{x}; \theta_r) = g(f(\boldsymbol{x}; \theta_f)_i; \theta_g).$$

The function $f(\cdot; \theta_f)$ denotes a context fusion layer, e.g., Bi-LSTM, Bi-GRU, etc., producing context-aware representation for each x_i. Then, $g(\cdot; \theta_g)$ maps $f(\cdot; \theta_f)$ to the probability of selecting the token. Note we can sample all z_i for different i in parallel because the probability of z_i (i.e., whether x_i is selected) does not depends on z_{i-1}. This is because the context features given by $f(\cdot; \theta_f)$ already take the sequential information into account, so the conditionally independent sampling does not discard any useful information.

To fully explore the high parallelizability of attention, we avoid using recurrent models in this paper. Instead we apply a more efficient $f(\cdot; \theta_f)$ inspired by source2token self-attention and intra-attention [Liu *et al.*, 2016], i.e.,

$$f(\boldsymbol{x}; \theta_f)_i = [x_i; \text{pooling}(\boldsymbol{x}); x_i \odot \text{pooling}(\boldsymbol{x})], \qquad (6)$$

$$g(h_i; \theta_g) = \text{sigmoid}(w^T \sigma(W^{(R)} h_i + b^{(R)}) + b), \qquad (7)$$

where $\odot$ denotes the element-wise product, and the $\text{pooling}(\cdot)$ represents the mean-pooling operation along the sequential axis. RSS selects a subset of tokens by sampling z_i according to the probability given by $g(h_i; \theta_g)$ for all $i = 1, 2, \ldots, n$ in parallel.

For the training of RSS, there are no ground truth labels to indicate whether or not a token should be selected, and the discrete random variables in $\boldsymbol{z}$ lead to a non-differentiable objective function. Therefore, we formulate learning the RSS parameter θ_r as a reinforcement learning problem, and apply the policy gradient method. Further details on the model training are presented in Section 4.

3.2 Reinforced Self-Attention (ReSA)

The fundamental idea behind this paper is that the hard and soft attention mechanisms can mutually benefit each other to overcome their inherent disadvantages via interaction within an integrated model. Based on this idea, we develop a novel self-attention termed ReSA. On the one hand, the proposed RSS provides a sparse mask to a self-attention module that only needs to model the dependencies for the selected token pairs. Hence, heavy memory loads and computations associated with soft self-attention can be effectively relieved. On the other hand, ReSA uses the output of the soft self-attention module for prediction, whose correctness (as compared to the ground truth) is used as reward signal to train the RSS. This alleviates the difficulty of training hard attention module.
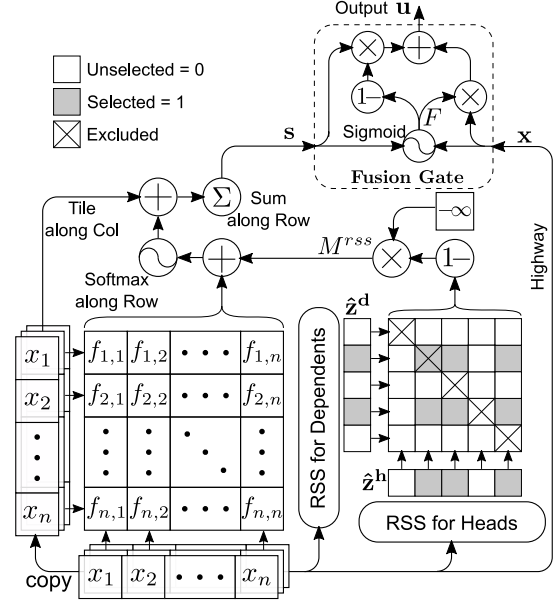

Figure 1: Reinforced self-attention (ReSA) model. $f_{i,j}$ denotes the alignment score obtained from $f(x_i, x_j)$.

Figure 1 shows the detailed architecture of ReSA. Given the token embedding in an input sequence, $\boldsymbol{x} = [x_1, \ldots, x_n]$, ReSA aims to produce token-wise context-aware representations, $\boldsymbol{u} = [u_1, \ldots, u_n]$. Unlike previous self-attention mechanisms, ReSA only selects a subset of head tokens, and generates their context-aware representations by only relating each head token to a small subset of dependent tokens. This notion is based on the observation that for many NLP tasks, the final prediction only relies on a small set of key words and their contexts, and each key word only depends on a small set of other words. Namely, the dependencies between tokens from the same sequence are sparse.

In ReSA, we use two RSS modules, as outlined in Section 3.1, to generate two sequences of labels for the selections of head and dependent tokens, respectively, i.e.,

$$\hat{\boldsymbol{z}}^{\boldsymbol{h}} = [\hat{z}_1^h, \ldots, \hat{z}_n^h] \sim \text{RSS}(\boldsymbol{x}; \theta_{rh}), \qquad (8)$$

$$\hat{\boldsymbol{z}}^{\boldsymbol{d}} = [\hat{z}_1^d, \ldots, \hat{z}_n^d] \sim \text{RSS}(\boldsymbol{x}; \theta_{rd}), \qquad (9)$$

We use $\hat{\boldsymbol{z}}^{\boldsymbol{h}}$ and $\hat{\boldsymbol{z}}^{\boldsymbol{d}}$ sampled from the two independent (parameter untied) RSS to generate an $n \times n$ mask M^{rss}, i.e.,

$$M_{ij}^{rss} = \begin{cases} 0, & \hat{z}_i^d = \hat{z}_j^h = 1 \ \& \ i \neq j \\ -\infty, & \text{otherwise.} \end{cases} \qquad (10)$$

The resulting mask is then applied as an extra mask to the masked self-attention mechanism introduced in Section 2.2. Specifically, we add M^{rss} to Eq.(4) and use

$$f^{rss}(x_i, x_j) = f(x_i, x_j) + M_{ij}^{rss} \qquad (11)$$

to generate the alignment scores. For each head token x_j, a softmax function is applied to $f^{rss}(\cdot, x_j)$, which produces a categorical distribution over all dependent tokens, i.e.,

$$P^j = \text{softmax}([f^{rss}(x_i, x_j)]_{i=1}^n), \text{ for } j = 1, \dots, n. \quad (12)$$

The context features of x_j is computed by

$$s_j = \sum_{i=1}^{n} P_i^j \odot x_i, \text{ for } j = 1, \dots, n, \qquad (13)$$

where $\odot$ denotes a broadcast product in the vanilla attention or an element-wise product in the multi-dim attention.

For a *selected* head token, as formulated in Eq.(10), the attention from a token to itself is disabled in M^{rss}, so the s_j for the selected head token encodes only the context features but not the desired context-ware embedding. For an *unselected* head token x_j with $\hat{z}_j^h = 0$, its alignment scores over all dependent tokens are equal to $-\infty$, which leads to the equal probabilities in P^j produced by the softmax function. Hence, s_j for each unselected token x_j can be regarded as the result of mean-pooling over all dependent tokens.

To merge the word embedding with its context feature for the *selected* heads, and distinguish the representations from others for the *unselected* heads, a fusion gate is used to combine s with the input embedding x in parallel and generate the final context-aware representations for all tokens, i.e.,

$$F = \text{sigmoid}\left(W^{(f)}[\boldsymbol{x}; \boldsymbol{s}] + b^{(f)} \right), \qquad (14)$$

$$\boldsymbol{u} = F \odot \boldsymbol{x} + (1 - F) \odot \boldsymbol{s}, \qquad (15)$$

where $W^{(f)}$, $b^{(f)}$ are the learnable parameters. The context-aware representations, $\boldsymbol{u} = [u_1, \dots, u_n]$, are final output. One primary advantage of ReSA is that it generates better predictions using less time and memory than existing self-attention mechanisms. In particular, major computations of ReSA are 1) the inference of self-attention over a shorter subsequence, and 2) the mean-pooling over the remaining elements. This is much more time- and memory- efficient than computing the self-attention over the entire input sequence.

3.3 Applications of the Proposed Models

To adapt ReSA for sentence encoding tasks, we build an RNN/CNN-free network, called reinforced self-attention network (ReSAN), which is solely based on ReSA and source2token self-attention (Section 2.2). In particular, we pass the output sequence of ReSA into a source2token self-attention module to generate a compressed vector representation, $e \in \mathbb{R}^{d_e}$, which encodes the semantic and syntactic knowledge of the input sentence and can be used for various downstream NLP tasks.

Further, we propose two simplified variants of ReSAN with a simpler structure or fewer parameters, i.e., 1) **ReSAN w/o unselected heads** which only applies the soft self-attention

to the selected head and dependent tokens, and 2) **ReSAN w/o dependency restricted** which use only one RSS to select tokens for both heads and dependents. Both variants entirely discard the information of the unselected tokens and hence are more time-efficient. However, neither can be used for context fusion, because the input and output sequences are not equal in length.

4 Model Training

The parameters in ReSAN can be divided into two parts, θ_r for the RSS modules and θ_s for the rest parts which includes word embeddings, soft self-attention module, and classification/regression layers. Learning θ_s is straightforward and can be completed by back-propagation in an end-to-end manner. However, Optimizing θ_r is more challenging because the RSS modules contain discrete variables $\boldsymbol{z}$ and, thus, the objective function is non-differentiable w.r.t. θ_r.

In supervised classification settings, we use the cross-entropy loss plus L2 regularization penalty as the loss, i.e.,

$$J_s(\theta_s) = \mathbb{E}_{(\boldsymbol{x}^*, y^*) \sim \mathcal{D}}[p(y = y^* | \boldsymbol{x}^*; \theta_s, \theta_r)] + \gamma \|\theta_s\|^2, \text{ (16)}$$

where $(\boldsymbol{x}^*, y^*)$ denotes a sample from dataset $\mathcal{D}$. The loss above is used for learning θ_s by back-propagation algorithm.

Optimizing θ_r is formulated as a reinforcement learning problem solved by the policy gradient method (i.e., REINFORCE algorithm). In particular, RSS plays as an agent and takes *action* of whether to select a token or not. After going through the entire sequence, it receives a loss value from the classification problem, which can be regarded as the negative delay *reward* to train the agent. Since the overall goal of RSS is to select a small subset of tokens for better efficiency and meanwhile retain useful information, a penalty limiting the number of selected tokens is included in the reward $\mathcal{R}$, i.e.,

$$\mathcal{R} = p(y = y^* | \boldsymbol{x}^*; \theta_s, \theta_r) + \lambda \sum \hat{z}_i / len(\boldsymbol{x}^*), \qquad (17)$$

where λ is the penalty weight and is fine-tuned with values from $\{0.005, 0.01, 0.02\}$ in all experiments. Then, the objective of learning θ_r is to maximize the expected reward, i.e.,

$$J_r(\theta_r) = \mathbb{E}_{(\boldsymbol{x}^*, y^*) \sim \mathcal{D}}\{\mathbb{E}_{\hat{\boldsymbol{z}}}[\mathcal{R}]\} \approx \frac{1}{N} \sum_{\boldsymbol{x}^*, y^*} \mathbb{E}_{\hat{\boldsymbol{z}}}[\mathcal{R}] \quad (18)$$

where the $\hat{\boldsymbol{z}} = (\hat{\boldsymbol{z}}^h, \hat{\boldsymbol{z}}^d) \sim p(\boldsymbol{z}^h | \boldsymbol{x}^*; \theta_{rh}) p(\boldsymbol{z}^d | \boldsymbol{x}^*; \theta_{rd}) \triangleq \pi(\hat{\boldsymbol{z}}; \boldsymbol{x}^*; \theta_r)$ and N is sample number in the dataset. Based on REINFORCE, the policy gradient of $J_r(\theta_r)$ w.r.t θ_r is

$$\nabla_{\theta_r} J_r(\theta_r) = \frac{1}{N} \sum_{\boldsymbol{x}^*, y^*} \sum_{\hat{\boldsymbol{z}}} \mathcal{R} \nabla_{\theta_r} \pi(\hat{\boldsymbol{z}}; \boldsymbol{x}^*; \theta_r) \qquad (19)$$

$$= \frac{1}{N} \sum_{\boldsymbol{x}^*, y^*} \mathbb{E}_{\hat{\boldsymbol{z}}}[\mathcal{R} \nabla_{\theta_r} \log \pi(\hat{\boldsymbol{z}}; \boldsymbol{x}^*; \theta_r)]. \qquad (20)$$

Although theoretically feasible, it is not practical to optimize θ_s and θ_r simultaneously, since the neural nets cannot provide accurate reward feedback to the hard attention at the beginning of the training phrase. Therefore, in early stage, the RSS modules are not updated, but rather forced to select all tokens (i.e., $\boldsymbol{z} = \boldsymbol{1}$). And, θ_s is optimized for several beginning epochs until the loss over development set does not

Model	$|\theta|$	T(s)/epoch	Inference T(s)	Train Accuracy	Test Accuracy
300D LSTM encoders [Bowman *et al.*, 2016]	3.0m			83.9	80.6
300D SPINN-PI encoders [Bowman *et al.*, 2016]	3.7m			89.2	83.2
600D Bi-LSTM encoders [Liu *et al.*, 2016]	2.0m			86.4	83.3
600D Bi-LSTM +intra-attention [Liu *et al.*, 2016]	2.8m			84.5	84.2
300D NSE encoders [Munkhdalai and Yu, 2017]	3.0m			86.2	84.6
600D Deep Gated Attn. [Chen *et al.*, 2017]	11.6m			90.5	85.5
600D Gumbel TreeLSTM encoders [Choi *et al.*, 2017b]	10m			93.1	86.0
600D Residual stacked encoders [Nie and Bansal, 2017]	29m			91.0	86.0
Bi-LSTM [Graves *et al.*, 2013]	2.9m	2080	9.2	90.4	85.0
Bi-GRU [Chung *et al.*, 2014]	2.5m	1728	9.3	91.9	84.9
Multi-window CNN [Kim, 2014]	1.4m	284	2.4	89.3	83.2
Hierarchical CNN [Gehring *et al.*, 2017]	3.4m	343	2.9	91.3	83.9
Multi-head [Vaswani *et al.*, 2017]	2.0m	345	3.0	89.6	84.2
DiSAN [Shen *et al.*, 2017a]	2.4m	587	7.0	91.1	85.6
300D ReSAN	3.1m	622	5.5	92.6	**86.3**

Table 1: Experimental results for different methods on SNLI. $|\theta|$: the number of parameters (excluding word embedding part). **T(s)/epoch**: average training time (second) per epoch. **Inference T(s)**: average inference time (second) for all dev data on SNLI with a batch size of 100.

decrease significantly. The resulting ReSAN now can provide a solid environment for training RSS modules through reinforcement learning. θ_r and θ_s are then optimized simultaneously to pursue a better performance by selecting critical token pairs and exploring their dependencies.

Training Setup: All experiments are conducted in Python with Tensorflow and run on a single Nvidia GTX 1080Ti. We use Adadelta [Zeiler, 2012] as optimizer, which performs more stable than Adam [Kingma and Ba, 2015] on ReSAN. All weight matrices are initialized by Glorot Initialization [Glorot and Bengio, 2010] and the biases are initialized as zeros. We use 300D GloVe 6B pre-trained vectors [Pennington *et al.*, 2014] to initialize the word embeddings x. The words which do not appear in GloVe from the training set are initialized by sampling from uniform distribution between $[-0.05, 0.05]$. We choose Dropout [Srivastava *et al.*, 2014] keep probability from $\{0.65, 0.70, 0.75, 0.8\}$ for all models and report the best result. The weight decay factor γ for L2 regularization is set to 5×10^{-5}. The number of hidden units is 300. We use ReLU [Glorot *et al.*, 2011] for all unspecified activation functions.

5 Experiments

We implement ReSAN, its variants and baselines on two NLP tasks, language inference in Section 5.1 and semantic relatedness in Section 5.2. A case study is then given to provide the insights into model. The baselines are listed as follows.

- **Bi-LSTM**: 600D bi-directional LSTM (300D forward LSTM + 300D backward LSTM) [Graves *et al.*, 2013];

- **Bi-GRU**: 600D bi-directional GRU [Chung *et al.*, 2014];

- **Multi-window CNN**: 600D CNN sentence embedding model (200D for each of 3, 4, 5-gram) [Kim, 2014];

- **Hierarchical CNN**: 3-layer 300D CNN [Gehring *et al.*, 2017] with kernel length 5. GLU [Dauphin *et al.*, 2016] and residual connection [He *et al.*, 2016b] are applied.

- **Multi-head**: 600D multi-head attention (8 heads, each has 75 hidden units), where the positional encoding method is applied to the input [Vaswani *et al.*, 2017].

- **DiSAN**: 600D directional self-attention network (forward+backward masked self-attn.) [Shen *et al.*, 2017a].

5.1 Natural Language Inference

The goal of natural language inference is to infer the semantic relationship between a pair of sentences, i.e., a premise and the corresponding hypothesis. The possible relationships are *entailment*, *neutral* or *contradiction*. This experiment is conducted on the Stanford Natural Language Inference [Bowman *et al.*, 2015] (SNLI)[1] dataset which consists of 549,367/9,842/9,824 samples for training/dev/test.

In order to apply sentence encoding model to SNLI, we follow Bowman *et al.* [2016] and use two parameter-tied sentence encoding models to respectively produce the premise and the hypothesis encodings, i.e., s^p, s^h. Their semantic relationship is represented by the concatenation of s^p, s^h, $s^p - s^h$ and $s^p \odot s^h$, which is passed to a classification module to generate a categorical distribution over the three classes.

The experimental results for different methods from leaderboard and our baselines are shown in Table 1. Compared to the methods from official leaderboard, ReSAN outperforms all the sentence encoding based methods and achieves the best test accuracy. Specifically, compared to the last best models, i.e., 600D Gumbel TreeLSTM encoders and 600D Residual stacked encoders, ReSAN uses far fewer parameters with better performance. Moreover, in contrast to the RNN/CNN based models with attention or memory module, ReSAN uses attention-only modules with equal or fewer parameters but outperforms them by a large margin, e.g., 600D Bi-LSTM + intra-attention (+3.0%), 300D NSE encoders (+1.7%) and 600D Deep Gated Attn (+0.8%). Furthermore, ReSAN even outperforms the 300D SPINN-PI encoders by 3.1%., which is

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[1]https://nlp.stanford.edu/projects/snli/

a recursive model and uses the result of an external semantic parsing tree as an extra input.

In addition, we compare ReSAN with recurrent, convolutional, and attention-only baseline models in terms of the number of parameters, training/inference time and test accuracy. Compared to the recurrent models (e.g., Bi-LSTM and Bi-GRU), ReSAN shows better prediction quality and more compelling efficiency due to parallelizable computations. Compared to the convolutional models (i.e., Multi-window CNN and Hierarchical CNN), ReSAN significantly outperforms them by 3.1% and 2.4% respectively due to the weakness of CNNs in modeling long-range dependencies. Compared to the attention-based models, multi-head attention and DiSAN, ReSAN uses a similar number of parameters with better test performance and less time cost.

Model	$|\theta|$	Inference T(s)	Test Accu.
ReSAN	3.1m	5.5	86.3
ReSAN w/o unselected heads	3.1m	5.3	86.1
ReSAN w/o dependency restricted	2.8m	4.6	85.6
ReSAN w/o hard attention	2.5m	7.0	86.0
ReSAN w/o soft self-attention	1.0m	1.6	83.4
ReSAN w/o all attentions	0.5m	1.8	83.1

Table 2: An ablation study of ReSAN.

Further, we conduct an ablation study of ReSAN, as shown in Table 2, to evaluate the contribution of each component. One by one, each component is removed and the changes in test accuracy are recorded. In addition to the two variants of ReSAN introduced in Section 3.3, we also remove 1) the hard attention module, 2) soft self-attention module and 3) both hard attention and soft self-attention modules. In terms of prediction quality, the results show that 1) the unselected head tokens do contribute to the prediction, bringing 0.2% improvement; 2) using separate RSS modules to select the head and dependent tokens improves accuracy by 0.5%; and 3) hard attention and soft self-attention modules improve the accuracy by 0.3% and 2.9% respectively. In terms of inference time, it shows that 1) the two variants are more time-efficient but have poorer performance; and 2) applying the RSS modules to self-attention or attention improves not only performance but also time efficiency.

5.2 Semantic Relatedness

Semantic relatedness aims to predict the similarity degree of a given pair of sentences, which is formulated as a regression problem. We use s^1 and s^2 to denote the encodings of the two sentences, and assume the similarity degree is a scalar between $[1, K]$. Following Tai *et al.* [2015], the relationship between the two sentences is represented as a concatenation of $s^1 \odot s^2$ and $|s^1 - s^2|$. The representation is fed into a classification module with K-way categorical distribution output. We implement ReSAN and baselines on the Sentences Involving Compositional Knowledge [Marelli *et al.*, 2014] (SICK) dataset, which provides the ground truth as similarity degree between $[1, 5]$. SICK come with a standard training/dev/test split of 4,500/500/4,927 samples.

Model	Pearson's r	Spearman's ρ	MSE
Meaning Factory[a]	.8268	.7721	.3224
ECNU[b]	.8414	/	/
DT-RNN[c]	.7923 (.0070)	.7319 (.0071)	.3822 (.0137)
SDT-RNN[c]	.7900 (.0042)	.7304 (.0042)	.3848 (.0042)
Cons. Tree-LSTM[d]	.8582 (.0038)	.7966 (.0053)	.2734 (.0108)
Dep. Tree-LSTM[d]	.8676 (.0030)	.8083 (.0042)	**.2532 (.0052)**
Bi-LSTM	.8473 (.0013)	.7913 (.0019)	.3276 (.0087)
Bi-GRU	.8572 (.0022)	.8026 (.0014)	.3079 (.0069)
Multi-window CNN	.8374 (.0021)	.7793 (.0028)	.3395 (.0086)
Hierarchical CNN	.8436 (.0014)	.7874 (.0022)	.3162 (.0058)
Multi-head	.8521 (.0013)	.7942 (.0050)	.3258 (.0149)
DiSAN	.8695 (.0012)	.8139 (.0012)	.2879 (.0036)
ReSAN	**.8720 (.0014)**	**.8163 (.0018)**	*.2623 (.0053)*

Table 3: Experimental results for different methods on SICK semantic relatedness dataset. The reported accuracies are the mean of five runs (standard deviations in parentheses). Cons. and Dep. represent Constituency and Dependency, respectively. [a][Bjerva *et al.*, 2014], [b][Zhao *et al.*, 2014], [c][Socher *et al.*, 2014], [d][Tai *et al.*, 2015]

The results in Table 3 show that the ReSAN achieves state-of-the-art performance for all three metrics. Particularly, ReSAN outperforms the feature engineering method by a large margin, e.g., Meaning Factory and ECNU. ReSAN also significantly outperforms the recursive models, which is widely used in semantic relatedness task, especially ones that demand external parsing results, e.g., DT/SDT-RNN and Tree-LSTMs. Further, ReSAN achieves the best results among all the recurrent, convolutional and self-attention models listed as baselines. This thoroughly demonstrates the capability of ReSAN in context fusion and sentence encoding.

5.3 Case Study

To gain an insights into how the hard/soft attention and fusion gate work within ReSA, we visualize their resulting values in this section. Note that only the values at token level are illustrated. If the attention probabilities and the gate values are feature-level, we average the probabilities over all features.

Two sentences from the SNLI test set serve as examples for this case study: 1) "*The three men sit and talk about their lives.*" and 2) "*A group of adults are waiting for an event.*".

The head and dependent tokens selected by RSS modules are show in Figure 2 (a small square with color white denotes unselection and vice versa). It shows that more dependent tokens are selected than the head tokens, because all non-trivial dependents should be retained to adequately modify the corresponding heads, e.g., *three, their* in sentence 1 and *group* in sentence 2, whereas only the key heads should be kept to compose the trunk of a sentence. It also shows that most stop words (i.e., articles, conjunctions, prepositions, etc.) are selected as neither head tokens nor dependent tokens.

We also visualize the probability distributions of the soft self-attention module in Figure 2 (the depth of color blue). From the figure, we observe that 1) the semantically important words (e.g., noun and verb) usually receive great attention from all the other tokens, e.g., *sit, talk, lives* in sentence 1 and *adults, waiting, event* in sentence 2; and 2) the atten-
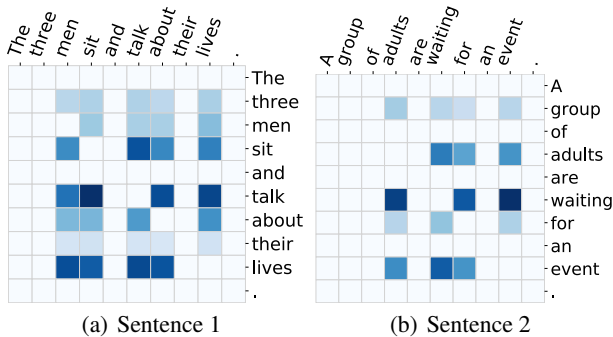
Figure 2: Attention probabilities of soft self-attention in ReSA. The tokens aligned in horizontal axis are heads, and the tokens aligned in vertical axis are dependents.

tion score increases if the token pair can be constituted to a sense-group, e.g., (*sit*, *talk*) in sentence 1 and (*adults*, *waiting*), (*waiting*, *event*) in sentence 2.
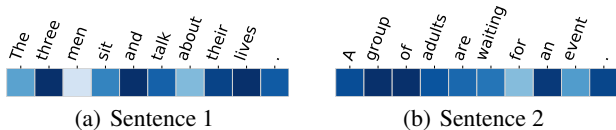

Figure 3: Fusion gate values in ReSA.

As a final step, we visualize the fusion gate values F in Figure 3, which combines the context features s with the original input x. The gate tends to select x rather than s if the value of F is large. The figure shows that, 1) the contextual features (i.e., mean-pooling result) of *unselected* heads are identical and less expressive, so their gate values F are larger to emphasize their original input; and 2) the gate values of the *selected* heads are smaller, so the context features produced by the self-attention module play a more important role in ReSA.

6 Related Work

Applying reinforcement learning to natural language processing (NLP) tasks recently attracts enormous interest for two main purposes, i.e., optimizing the model according to non-differentiable objectives and accelerating the model speed. Lei *et al.* [2016] propose a method to select a subset of a review passage for sentiment analysis from a specific aspect. He *et al.* [2016a] use reinforcement learning method to fine-tune a bilingual machine translation model by well-trained monolingual language models. Yogatama *et al.* [2016] use built-in transition-based parsing module to generate semantic constituency parsing tree for downstream NLP tasks by using reinforcement learning. Yu *et al.* [2017] propose a reinforcement learning based skim reading method, which is implemented on recurrent models, to skim the insignificant time slots to achieve higher time efficiency. Choi *et al.* [2017a] separately implement a hard attention or a soft attention on a question answering task to generate the document summary. Shen *et al.* [2017b] use reinforcement learning method to at-

tend the memory with dynamic episode number rather than fixed one for adequate and efficient machine comprehension. Hu *et al.* [2017] employ policy gradient method to optimize the model with non-differentiable objective of machine comprehension, i.e., F1 score of matching the prediction with the ground truth. Li *et al.* [2017] propose a service dialogue system to sell movie tickets online, in which the agent in reinforcement learning is used to select which user's information should be obtained in next dialogue round for minimum number of dialogue rounds to sell the ticket successfully. Zhang and Lapata [2017] simplify a sentence with objectives of maximum simplicity, relevance and fluency, where all three objectives are all non-differentiable w.r.t the parameters of model.

Hard attention mechanisms are proposed to alleviate the weakness of soft attention mechanisms, which are separately applied to computer vision (CV) or NLP tasks in existing works. The hard attention mechanism is first proposed for visual question answer task [Xu *et al.*, 2015] and empirically outperform the soft attention, where the hard attention is used to focus on a particular, small and local image region for a time slot of a recurrent model, whose output is used to compose the answer sentence. Gulcehre *et al.* [2016] propose a dynamic neural Turing machine, which is implemented with both continuous (differentiable) and discrete (non-differentiable) memory read/write approaches. Aharoni *et al.* [2017] present a neural model for morphological inflection generation, where a hard attention mechanism is used to align the characters in a word with its inflection because the inflection mapping is nearly-monotonic. Additionally, Aharoni *et al.* [2017] point out the defects of both hard and soft attention in memory networks, and propose a hierarchical memory network rather than an actual hybrid of soft and hard attention to alleviate those defects.

7 Conclusions

This study presents a context fusion model, reinforced self-attention (ReSA), which naturally integrates a novel form of highly-parallelizable hard attention based on reinforced sequence sampling (RSS) and soft self-attention mechanism for the mutual benefit of overcoming the intrinsic weaknesses associated with hard and soft attention mechanisms. The hard attention modules could be used to trim a long sequence into a much shorter one and encode rich dependencies information for a soft self-attention mechanism to process. Conversely, the soft self-attention mechanism could be used to provide a stable environment and strong reward signals, which improves the feasibility of training the hard attention modules.

Based solely on ReSA and a source2token self-attention mechanism, we then propose an RNN/CNN-free attention model, reinforced self-attention network (ReSAN), for sentence encoding.

Experiments on two NLP tasks – natural language inference and semantic relatedness – demonstrate that ReSAN deliver a new best test accuracy for the SNLI dataset among all sentence-encoding models and state-of-the-art performance on the SICK dataset. Further, these results are achieved with equal or fewer parameters and in less time.

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A Comparison to a Iterative Sampling

To verify the RSS that uses parallel discrete sampling is sufficient to trim the long sentence and model the dependencies, we implement the iteration-based sequence sampling method following Lei *et al.* [2016] and integrate it with the soft self-attention in the same way as ReSA.

Given a input sequence, $\boldsymbol{x} = [x_1, \ldots, x_n]$, iterative sampling aims to learn the following product distribution.

$$p(\boldsymbol{z}|\boldsymbol{x}; \theta_r) = \prod_{i=1}^{n} p(z_i|\boldsymbol{x}; z_{1:i-1}; \theta_r). \quad (21)$$

A RNN is used to parameterize the conditional probability function above and the basic RNN rather than LSTM or GRU is employed to reduce the number of parameters. The latent state of the RNN can be referred to as the embedding of both contextual information and history selection results. The recurrence can be formally written as

$$p_i = \text{sigmoid}(w^T \sigma(W^{(p)}[h_{i-1}; x_i] + b^{(p)}) + b), \quad (22)$$
$$z_i \sim p_i, \quad (23)$$
$$x'_i = [x_i; z_i], \quad (24)$$
$$h_i = \text{RNN}(h_{i-1}, x'_i; \theta_{rnn}), \quad (25)$$

where $\sim$ denotes the discrete sampling operation and θ_{rnn} is the learnable parameters of RNN. Consequently, after this recurrence over the input sequence, a sequence of sampling result, $\boldsymbol{z} = [z_1, \ldots, z_n]$, is obtained, which shares the same notion with RSS.

We then apply two iterative sampling modules which make selections over the dependent and head tokens, respectively. The output of these two sampling modules is formated as a mask which is then applied to the compatibility function of soft self-attention mechanism. The details of the integration are described in the main paper.

For the comparison of RSS and iterative sampling, we also implement the ReSAN with iterative sampling on SNLI dataset that is one of the largest NLP dataset designed to test the sentence-encoding model. A thorough comparison of them in terms of parameters number, training/inference time, training/test accuracy are show in Table 4

	ReSAN w/ RSS	ReSAN w/ Iteration
Parameter Num (300D)	*3.1m*	4.0m
Time/Epoch	*622s*	2996s
Inference Time	*5.5s*	17.1s
Train Accuracy	92.6%	92.3%*
Test Accuracy	86.3%	86.2%*

Table 4: A thorough comparison of a ReSAN with RSS and Iterative Sampling on SNLI dataset. *The accuracies of these two models should be experimentally equal, but, due to the randomness of neural networks (e.g., initialization, batch SGD), there are some experimental error on the accuracies.

As shown in the table, compared with ReSAN with iterative sampling, the one with RSS requires much fewer parameters, $5\times$ less training time and $3\times$ less inference time to achieve the competitive test accuracy. This is consistent with the motivation and target for which we develop the RSS.

B A Full Background of Soft Attention

We give a full background of soft attention mechanisms for readers to comprehend these mechanisms in depth. All attention mechanisms introduced in this section are designed for natural language processing tasks, whose the handling object is a natural language sentence (i.e., a sequence of ordered tokens).

B.1 Vanilla Attention Mechanism

Vanilla/traditional attention mechanism is first proposed by Bahdanau *et al.* [2015]. Given a sequence of embedded input tokens, $\boldsymbol{x} = [x_1, \ldots, x_n] \in \mathbb{R}^{d_e \times n}$, and a vector representation of query, $q \in \mathbb{R}^{d_q}$, attention mechanism computes the alignment score between x_i and q by a compatibility function $f(x_i, q)$, which measures the dependency/relevance/similarity between x_i and q, or the attention of q to x_i. A softmax function is then applied to all the alignment scores, $[f(x_i, q)]_{i=1}^{n}$, to generate categorical a probability distribution, $p(z|\boldsymbol{x}, q)$, by normalizing the scores over all the n tokens of $\boldsymbol{x}$. Here, z is a random variable indicating which token in $\boldsymbol{x}$ is important to q for a specific task. Namely, a large $p(z = i|\boldsymbol{x}, q)$ means x_i could contribute important information to q. These processes can be formulated by

$$a = [f(x_i, q)]_{i=1}^{n}, \quad (26)$$
$$p(z|\boldsymbol{x}, q) = \text{softmax}(a). \quad (27)$$

The softmax function is always implemented over the sequential or temporal axis, and the probability $p(z = i|\boldsymbol{x}, q)$ can be detailedly written as

$$p(z = i|\boldsymbol{x}, q) = \frac{\exp(f(x_i, q))}{\sum_{i=1}^{n} \exp(f(x_i, q))}. \quad (28)$$

The output of vanilla attention mechanism is a weighted sum of the embeddings for all tokens in $\boldsymbol{x}$, where the weights are given by $p(z|\boldsymbol{x}, q)$. Consequently, this mechanism can be written as the expectation of a token sampled according to its importance, i.e.,

$$s = \sum_{i=1}^{n} p(z = i|\boldsymbol{x}, q)x_i = \mathbb{E}_{i \sim p(z|\boldsymbol{x}, q)}(x_i), \quad (29)$$

where $s \in \mathbb{R}^{d_e}$ can be used as the context features of query q in light of the sequence $\boldsymbol{x}$, or sentence encoding of $\boldsymbol{x}$.

There are mainly two kinds of **compatibility functions**: one is the additive compatibility function leading to the *additive or multi-layer perceptron attention mechanisms*, and another is multiplicative compatibility function leading to *multiplicative or dot-product attention mechanisms*. In particular, additive attention mechanisms [Bahdanau *et al.*, 2015; Shang *et al.*, 2015] and multiplicative attention mechanisms [Vaswani *et al.*, 2017; Sukhbaatar *et al.*, 2015; Rush *et al.*, 2015] share the same form of processes of vanilla attention mechanism introduced above, but are different in the compatibility function $f(x_i, q)$. The additive attention mechanisms are associated with

$$f(x_i, q) = w^T \sigma(W^{(1)}x_i + W^{(2)}q) \quad (30)$$

where $W^{(1)} \in \mathbb{R}^{d_h \times d_e}, W^{(2)} \in \mathbb{R}^{d_h \times d_q}, w \in \mathbb{R}^{d_h}$ are the learnable parameters, and $\sigma(\cdot)$ denotes the activation function. The multiplicative attention mechanisms, however, use inter product or cosine similarity as the $f(x_i, q)$, i.e.,

$$f(x_i, q) = \left\langle W^{(1)} x_i, W^{(2)} q \right\rangle. \qquad (31)$$

In practice, the additive attention mechanisms empirically outperform the multiplicative ones in prediction performance, but the latter ones are faster and more memory-efficient due to less matrix multiplication computation involved [Britz *et al.*, 2017; Vaswani *et al.*, 2017; Shen *et al.*, 2017a].

B.2 Multi-dim Attention Mechanism

Multi dimensional attention (multi-dim attention) mechanism is a natural extension of the vanilla attention mechanism with additive compatibility function. Instead of computing a single scalar score $f(x_i, q)$ for each token x_i as shown in Eq.(30), multi-dim attention mechanism computes a feature-wise score vector for x_i by replacing weight vector w in Eq.(30) with a matrix W, i.e.,

$$f(x_i, q) = W^T \sigma \left(W^{(1)} x_i + W^{(2)} q \right), \qquad (32)$$

where $f(x_i, q) \in \mathbb{R}^{d_e}$ is a vector with the same length as x_i, and $W \in \mathbb{R}^{d_h \times d_e}$. Further two bias terms are added to the parts in and out activation function $\sigma(\cdot)$, i.e.,

$$f(x_i, q) = W^T \sigma \left(W^{(1)} x_i + W^{(2)} q + b^{(1)} \right) + b. \qquad (33)$$

Then, a categorical distribution $p(z_k | \boldsymbol{x}, q)$ is computed over all the n tokens for each feature $k \in [d_e]$. A large $p(z_k = i | \boldsymbol{x}, q)$ means that feature k of token i is important to q.

The same procedure Eq.(26)-(28) in vanilla attention mechanism is applied to the kth dimension of $f(x_i, q)$. In particular, for each feature $k \in [d_e]$, $f(x_i, q)$ is replaced with $[f(x_i, q)]_k$, and z is changed to z_k in Eq.(26)-(28). Now, each feature k in each token i has an importance weight $P_{ki} \triangleq p(z_k = i | \boldsymbol{x}, q)$. The output of multi-dim attention mechanism s is written as

$$s = \left[\sum_{i=1}^n P_{ki} \boldsymbol{x}_{ki} \right]_{k=1}^{d_e} = \left[\mathbb{E}_{i \sim p(z_k | \boldsymbol{x}, q)} (\boldsymbol{x}_{ki}) \right]_{k=1}^{d_e}. \qquad (34)$$

The output of multi-dim attention mechanism can also be written as an element-wise product, i.e., $s = \sum_{i=1}^n P_{\cdot i} \odot x_i$.

The word embedding usually suffers from the polysemy in natural language. Since vanilla attention mechanism computes a single importance score for each word based on the word embedding, it cannot distinguish the meanings of the same word in different contexts. Multi-dim attention mechanism, however, computes a score for each feature of each word, so it can select the features that can best describe the word's specific meaning in any given context, and include this information into the output s.

B.3 Self-Attention Mechanism

Self-attention mechanisms are special cases of the attention mechanism where the query q stems from the input sequence itself. Hence, self-attention mechanisms can model the dependencies between tokens from the same sequence. Recently, a variety of self-attention mechanisms have been developed, each serving a distinct purpose, but most can be roughly categorized into two types, token2token self-attention mechanism and source2token self-attention mechanism.

Token2token self-attention mechanism: token2token self-attention mechanisms aim to produce a context-aware representation for each token in light of its dependencies on other tokens in the same sequence. The query q is replaced with the token x_j, and the dependency of x_j on another token x_i is computed by $f(x_i, x_j)$. There are two proposed self-attention mechanisms in this type, i.e., **scaled dot-product attention** which composes the *multi-head attention* [Vaswani *et al.*, 2017] and **masked self-attention** which leads to *directional self-attention* [Shen *et al.*, 2017a].

1) **Scaled dot-product attention mechanism**: In general cases, this mechanism requires three input arguments, i.e., a query sequence $\boldsymbol{q} \in \mathbb{R}^{d_k \times m}$, a key sequence $\boldsymbol{k} \in \mathbb{R}^{d_k \times n}$, and a value sequence $\boldsymbol{v} \in \mathbb{R}^{d_v \times n}$ that is associated with the key sequence. Given a token x_i from $\boldsymbol{k}$ and a token x_j from $\boldsymbol{q}$, the compatibility function $f(x_i, x_j)$ is computed to produce a scaled dot-product similarity of x_i and x_j. The output sequence, $\boldsymbol{s} = [s_1, \ldots, s_n]$, is computed as

$$\boldsymbol{s} = \text{dpAttention}(\boldsymbol{q}, \boldsymbol{k}, \boldsymbol{v}) = \boldsymbol{v} \, \text{softmax}(\frac{\boldsymbol{q}^T \boldsymbol{k}}{\sqrt{d_k}})^T. \qquad (35)$$

In a specific case of this scaled dot-product self-attention, the three input arguments are identical, i.e., $\boldsymbol{q} = \boldsymbol{k} = \boldsymbol{v} = [x_1, \ldots, x_n] \in \mathbb{R}^{d_e \times n}$. As for **multi-head attention mechanism**, the input sequence is projected onto multiple subspaces, then scaled dot-product attention is applied to the representations in each subspace. As a last step, the output is concatenated into the final output $\boldsymbol{s}$ as

$$\boldsymbol{s} = \text{concat}(H_1; \ldots; H_h), \qquad (36)$$

$$\text{where } H_i = \text{dpAttention}(W_i^q \boldsymbol{q}, W_i^k \boldsymbol{k}, W_i^v \boldsymbol{v},). \qquad (37)$$

2) **Masked self-attention mechanism**: This mechanism is more sophisticated than scaled dot-product attention in that, it uses multi-dim and multi-layer perceptron with an additional position mask, rather than a scaled dot-product, as the compatibility function, i.e.,

$$f(x_i, x_j) =$$
$$c \cdot \tanh \left([W^{(1)} x_i + W^{(2)} x_j + b^{(1)}]/c \right) + M_{ij}, \qquad (38)$$

where c is a scalar and M is the mask with each entry $M_{ij} \in \{-\infty, 0\}$. When $M_{ij} = -\infty$, applying the softmax function to a results in a zero probability, $p(z = i | \boldsymbol{x}, x_j) = 0$, which switches off the attention of x_j to x_i. An asymmetric mask where $M_{ij} \neq M_{ji}$ enforces directional attention between x_i and x_j, which can encode temporal order information. Two positional masks have been designed to encode the forward and backward temporal order, respectively, i.e.,

$$M_{ij}^{fw} = \begin{cases} 0, & i < j \\ -\infty, & \text{otherwise} \end{cases} \qquad M_{ij}^{bw} = \begin{cases} 0, & i > j \\ -\infty, & \text{otherwise} \end{cases}$$

Name	Purpose	Query Source	Compatibility Function
Vanilla attention [Bahdanau *et al.*, 2015]	Compression	Exterior	Additive/Multiplicative
Multi-dim attention [Shen *et al.*, 2017a]	Compression	Exterior	Additive
Self-alignment attention [Hu *et al.*, 2017]	Context fusion	Interior	Multiplicative
Multi-head attention [Vaswani *et al.*, 2017]	Context fusion	Interior	Multiplicative
Masked self-attention [Shen *et al.*, 2017a]	Context fusion	Interior	Additive
Intra-attention [Liu *et al.*, 2016]	Compression	Interior	Multiplicative
multi-dim source2token attention [Shen *et al.*, 2017a]	Compression	Interior	Additive

Table 5: A summary of various soft attention mechanisms.

Given input sequence $\boldsymbol{x}$ and a mask M, every $f(x_i, x_j)$ is computed according to Eq.(4). Similar to P in multi-dim attention mechanism, we compute a probability matrix $P^j \in \mathbb{R}^{d_e \times n}$ for each x_j such that $P^j_{ki} \triangleq p(z_k = i | \boldsymbol{x}, x_j)$. The output with context features encoded for x_j is

$$s_j = \sum_{i=1}^{n} P^j_{\cdot i} \odot x_i \qquad (39)$$

The output of masked self-attention attention mechanism for all elements in $\boldsymbol{x}$ is $\boldsymbol{s} = [s_1, s_2, \ldots, s_n] \in \mathbb{R}^{d_e \times n}$.

In forward and backward masks, $M_{ii} = -\infty$. Thus, the attention of a token to itself is blocked, so the output of masked self-attention mechanism comprises the features of the context around each token rather than context-aware features. Hence, **directional self-attention mechanism** [Shen *et al.*, 2017a] is proposed to use a fusion gate to combine the embedding of each token with its context features. Specifically, a fusion gate combines the input and output of a masked self-attention to produce context-aware representations. This idea is similar to the highway network [Srivastava *et al.*, 2015]. The fusion gate is formally defined as

$$F = \text{sigmoid}\left(W^{(f1)}\boldsymbol{s} + W^{(f2)}\boldsymbol{x} + b^{(f)}\right) \qquad (40)$$

$$\boldsymbol{u} = F \odot \boldsymbol{x} + (1 - F) \odot \boldsymbol{s} \qquad (41)$$

where $W^{(f1)}, W^{(f2)} \in \mathbb{R}^{d_e \times d_e}$ and $b^{(e)} \in \mathbb{R}^{d_h}$ are the learnable parameters of the fusion gate. And the $\boldsymbol{u} = [u_1, \ldots, u_n]$ is the sequence of context-aware representations for corresponding tokens in the input sequence.

Source2token self-attention mechanism: The goal of this type of mechanisms is to generate a expressive sentence encoding for a sequence with semantic and syntactic knowledge embedded. This type of self-attention mechanism directly compresses a sequence into a vector representation calculated from the dependency between each token x_i and the entire source sequence $\boldsymbol{x}$. Hence, this form of self-attention mechanism is highly data- and task- driven.

There are also two proposed self-attention mechanisms in this type, i.e., **intra-attention mechanism** [Liu *et al.*, 2016] and **multi-dim source2token self-attention mechanism** [Shen *et al.*, 2017a].

1) **intra-attention mechanism** replaces the query q with the the result of mean-pooling over the input sequence. The compatibility function defined in Liu *et al.* [2016] is

$$f(x_i, \boldsymbol{x}) = w^T \tanh(W^{(1)}x_i + W^{(2)} \text{pooling}(\boldsymbol{x})), \quad (42)$$

where the alignment score is a scalar for each token. Then, the softmax function is applied over all the alignment score to produce the categorical distribution in the same way as the vanilla attention mechanism, which is formally defined in Eq.(26)-Eq.(28). Therefore, the output of this attention mechanism can be written as

$$s = \sum_{i=1}^{n} p(z = i | \boldsymbol{x}, q)x_i = \mathbb{E}_{i \sim p(z|\boldsymbol{x},q)}(x_i), \qquad (43)$$

which is usually used as the sentence encoding of the input token sequence $\boldsymbol{x}$.

2) **multi-dim source2token self-attention mechanism** directly removes the query q from the compatibility function defined in the multi-dim attention mechanism (Eq.(33)), i.e.,

$$f(x_i, q) = W^T \sigma\left(W^{(1)}x_i + b^{(1)}\right) + b. \qquad (44)$$

The probability matrix is defined as $P_{ki} \triangleq p(z_k = i | \boldsymbol{x})$ and is computed in the same way as P in the multi-dim attention mechanism. The output s is also same, i.e.,

$$s = \sum_{i=1}^{n} P_{\cdot i} \odot x_i \qquad (45)$$

B.4 Summary

We summarize the widely-used attention mechanisms via categorizing them into different classes, which are demonstrated in Table 5. By the *purposes*, the soft attention mechanisms could be coarsely categorized into two types: 1) context fusion and 2) sequence compression. By the *query sources*, the mechanisms could also be categorized into two types: 1) exterior (query from arbitrary source) and 2) interior (query from sequence itself). By the *compatibility functions*, the mechanisms could also be categorized into two types: 1) additive or multi-layer perceptron attention and 2) multiplicative or dot-product attention.