Learning for Expressive Task-Related Sentence Representations

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Abstract

NLP models learn sentence representations for downstream tasks by tuning a model which is pre-trained by masked language modeling. However, after tuning, the learned sentence representations may be skewed heavily toward label space and thus are not expressive enough to represent whole samples, which should contain task-related information of both sentence inputs and labels. In this work, we learn expressive sentence representations for supervised tasks which (1). contain task-related information in the sentence inputs, and (2). enable correct label predictions. To achieve this goal, we first propose a new objective which explicitly points out the label token space in the input, and predicts categories of labels via an added [MASK] token. This objective encourages fusing the semantic information of both the label and sentence. Then we develop a neighbor attention module, added on a frozen pretrained model, to build connections between label / sentence tokens via their neighbors. The propagation can be further guided by the regularization on neighborhood representations to encourage expressiveness. Experimental results show that, despite tuning only 5% additional parameters over a frozen pretrained model, our model can achieve classification results comparable to the SOTA while maintaining strong expressiveness as well.

1 Introduction

Learning expressive sentence representations — ones that contain task-related information from the input (e.g. rationales) for prediction — is desirable in many ways. Nudging models to learn representations that indicate rationales for the target labels can encourage the prediction based on proper reasoning using task-relevant information, rather than relying on spurious heuristics and artifacts (Camburu et al., 2018; Gururangan et al., 2018). If the expressive representations are also interpretable, they can help us better understand and guide the model behavior (Doshi-Velez and Kim, 2017; Lipton, 2018; DeYoung et al., 2019). Moreover, expressive representations may be useful in tasks such as contrastive learning (Giorgi et al., 2020; Wu et al., 2020; Gao et al., 2021), where the relative relationships between sample representations are crucial.

Standard fine-tuning approaches, however, may not usually yield expressive sentence representations. The fine-tuned sentence representations, typically packed in the [CLS] tokens, naturally skew heavily towards the label space, and away from the input semantics even if they are task-related. For example, consider a text-entailment sample \((s_1, s_2, y)\) where \(s_1 = \text{‘The man is exercising’}, s_2 = \text{‘The man is sleeping’}, y = \text{‘contradiction’}.\) After standard fine-tuning, the [CLS] token representation will usually be mapped to a space near \(y\) (or reflect categorical information when \(y\) is numerical). In contrast, an expressive representation should relate to the important words in the input sample such as ‘exercising’, ‘sleeping’, which provides essential task-related information that distinguishes it from other ‘contradiction’ samples. One way to avoid this issue is to train models using task-specific explanations or rationales (Camburu et al., 2018), when such data is available. In this work, we ask if we can learn representations that are both effective and expressive, but without relying on the extra training for explanations or rationales.

To learn such expressive sentence representations, we focus on both the task formulation and model design aspects. In standard fine-tuning, the classification objective with numerical labels does not include label tokens (e.g. ‘entailment’ or ‘contradiction’) in the task formulation, and thus the trained models do not necessarily learn to connect the semantics of label tokens to the sentence inputs, resulting in predictions that may not rely on true rationales. The recently introduced prompt-based methods target such semantic connections by re-
formulating classification problems into [MASK] token prediction problems to predict label tokens via carefully designed prompts (Liu et al., 2021a). However, by directly training [MASK] representations to predict label tokens, the learned representations may still skew heavily towards the label token space – they may contain information only about the word ‘contradiction’ rather than indicating ‘exercising’ and ‘sleeping’ are contradictions in the sample. In this work, we address this issue by introducing a new objective, in which we first add all label tokens as part of the input, then tune a [MASK] token representation to predict a numerical label. This allows the model to connect the input words to the label token space, but without skewing the [MASK] representation directly toward a specific label token.

On the modeling front, the key to expressive representations lies in learning semantic connections among labels and sentences. We establish such connections with the help of neighbors selected for each token, by learning new neighbor-based attention weights, on top of the standard self-attention weights. To learn generalized relationships among tokens, we keep the underlying pre-trained language model frozen (Houlsby et al., 2019). Our approach is similar in spirit to existing prompt tuning methods (Li and Liang, 2021; Lester et al., 2021), which can be viewed as establishing semantic connections by adding prompt tokens with trainable embeddings in inputs. One disadvantage of prompt tuning is that the learning of arbitrary, continuous prompt embeddings can be hard to regularize and less interpretable compared to discrete prompts (Lester et al., 2021). In our model, we control the learning by adding regularizations to limit the mobility of the neighborhood and encourage the expressiveness of the [MASK] representation.

Our contributions in this work are: (1) a task formulation to learn more expressive sentence representations, (2), a transformer with neighbor attention, and a regularization term to guide the training. With 5% parameters for training compared to fine-tuning, our model still achieves > 95% of the fine-tuning performance and moreover, learns more expressive sentence representations that close to rationale token representations for prediction.

2 Motivation

In this paper, our goal is to learn expressive sentence representations with the help of a frozen pre-trained language model. In particular, we want sentence representations to contain task-relevant information about the input sentences; specifically, to be close to representations of the rationale tokens for the input instances. In this section, we present the intuition behind our problem formulation for producing expressive representations, and establish both the connections and differences of our method to prompt tuning.

[MASK] instead of [CLS] for categorical label prediction The [CLS] token representations, which are commonly tuned for predicting categorical labels (e.g. 0, 1, 2...) of target tasks, are usually not pre-trained (Liu et al., 2019) or not pre-trained to capture semantic correlations among tokens at each input position (Devlin et al., 2018). On the other hand, the [MASK] token representations are pre-trained by masked language modeling to learn information from the other contextual tokens. This means the [MASK] token is directed to a representation space that is closer to related tokens in the input sentences as shown in Figure 1(a). This property of [MASK] token can encourage the model to consider semantic correlations among tokens in representation learning, which suits our goal.

We then have to learn semantic correlations among label tokens and sentences. With the standard training objective, the label token space (i.e. the space spanning the embeddings for the label tokens) is hidden from the model. In prompt tuning, by adding trainable embeddings (i.e. prompts) in the inputs and learning to predict label tokens, some of the prompts may be trained to be close to the implicit label space (as shown in Figure 1(b)). However, since the [MASK] representation is decoded to predict the label tokens, there’s no guarantee that it will contain token information from the input sentence. To learn representations that fuse information from both sentence and label semantics, we predict each sample’s categorical (numerical) label instead of label tokens from [MASK], with all label tokens (e.g. in the format of “entailment or contradiction”) given in inputs to explicitly point out the label token space (Fig. 1(c) upper left).

Neighborhood instead of arbitrary prompts From the model perspective, one problem of prompt tuning is that the learning of prompt embeddings is hard to control, and its capacity highly relies on the prompt length, whose optimal value varies from task to task (Liu et al., 2021b). In our
work, we build connections between label and sentence semantics via neighborhood tokens, which establish a ‘path’ between far away tokens. For the example given in Section 1, it may be hard to directly connect (‘exercising’, ‘sleeping’) with ‘contradiction’ with the pretrained model. But if ‘awake’, ‘opposite’ are in the neighborhood of ‘exercising’ and ‘contradiction’ respectively, the pretrained model may be able to first connect (‘awake’, ‘sleeping’) with ‘opposite’ and then to ‘contradiction’. Based on this, in specific layers we add neighbor-attentions in addition to the standard self-attention in order to inject token representations with neighborhood information. Furthermore, by promoting similarity between representations of neighboring tokens and [MASK] token through regularization, we can better control these connections to learn expressive [MASK] representations.

### 3 Task Formulation

For sentence-level classification tasks, we have i.i.d. samples \( \{ (x^{(i)}, y^{(i)}) \}_{i=1}^{N} \) drawn from a distribution \( \mathcal{D} \), where \( x \) represents an input sentence and \( y \) represents its label. More generally, \( x \) can also be a sentence pair \( x = [x_1, x_2] \) for pair-wise tasks such as textual entailment. In the traditional classification with \( p \) classes, \( y \) is in a set of categorical numbers \( \{1, 2, ..., p\} \). Recent work targets prediction of label tokens to learn sentence representations which are generalizable across tasks (Lester et al., 2021) and beneficial for few-shot learning (Brown et al., 2020; Gao et al., 2020). In such cases, labels are from a set \( \{Y_1, Y_2, ..., Y_p\} \) where each \( Y_i \) represents a label word. In some cases, a label word is decomposed into several tokens during tokenization, which may require text-to-text models like T5 (Raffel et al., 2019) for predictions.

In the typical fine-tuning setup, the input has a format of \([CLS] x_1 [SEP] x_2 [SEP]\), and the probability of the class labels \( y \) is predicted using the [CLS] representation. In the case of label token prediction, a [MASK] token is added in the input and its representation is used to predict \( Y \). In our work, to learn expressive sentence representations, we also utilize [MASK] for label predictions because it is pre-trained to capture contextual information. To inject label semantics into the sentence representations, we also add all the label tokens to the input. This can be seen as a prompt-based way of adding label semantics. So the input \( X \) in our objective has the format:

\[
[CLS] Y_1 \text{ or } Y_2 \text{ or } ... \text{ or } Y_p \text{ of } [MASK] [SEP] x_1 [SEP] x_2 [SEP], \tag{1}
\]

where we use ‘or’ to connect label words in \( \{Y\} \). This format can be used for any task where label words are available. To combine information from both the label tokens and sentences in the representation, we predict the categorical \( y \) from the [MASK] token representation. The training objective is:

\[
\max_{\theta} \mathbb{E}_{x,y \sim \mathcal{D}}[Pr_{\theta}(y|X)], \ y \in \{1, ..., p\} \tag{2}
\]

where \( \theta \) denotes the trainable parameters of the model.
where $d$ will be considered in self attentions on the $l$-th layer. The token embedding layer, which contains $e$ vocabulary size. We then randomly select $k$ bor representations from $e$ the embeddings are extracted from the vocabulary $W = 100$. Initial neighborhood. In this work, we set $k$ scores of $h$ as $n$ embeddings $h$ of all tokens from the vocabulary, can be used to get neighbors of each token. Denote the $n$ input token representations on the $l$-th layer as $h^{(l)} = [h_1^{(l)}, ..., h_n^{(l)}]$. After propagations over several layers, we still observe strong correlation between $h_i^{(l)}$ and $e$ at different layers of BERT-base (Appendix B), which may due to the residual connections (He et al., 2016) at each layer. In this case, we calculate similarities among the $i$-th input representation and token embeddings by:

$$\text{Sim}(e, h_i^{(l)}) = \exp(W_e(h_i^{(l)})^T / \sqrt{d_h}),$$

(3)

where $d_h$ represents the dim of representations, $h_i^{(l)} \in \mathbb{R}^{1 \times d_h}$, $W_e \in \mathbb{R}^{|V| \times d_h}$ is the matrix of a pretrained token embeddings, $|V|$ represents the vocabulary size. We then randomly select $k$ tokens out of $K$ candidates to be neighbors of $h_i^{(l)}$, where candidates are tokens with top-$K$ similarity scores of $h_i^{(l)}$. Here, $K$ controls the range of the initial neighborhood. In this work, we set $k = 10$, $K = 100$. The corresponding neighbor embeddings are extracted from the vocabulary $W_e$ with the $i$-th positional embedding added.

We then apply a transformation to transfer neighbor representations from $e$ space to $h$ space. For the $j$-th neighbor of $h_i^{(l)}$ with embedding $e_{ij}$, the new representation $m_{ij}^{(l)}$ is:

$$m_{ij}^{(l)} = \text{LN}_e(f_e(e_{ij} - e_i) + (e_{ij} - e_i) + h_i^{(l)}),$$

where $e_i$ is the embedding of the $i$-th input, $f_e$ is a linear function: $\mathbb{R}^{d_h} \rightarrow \mathbb{R}^{d_h}$, ‘LN’ represents $Layer\;\text{Norm}$. Better choices for this transformation may further benefit the representation learning, which we leave for future studies. After this step, neighbor representations of $h_i^{(l)}$ are denoted as $m_i^{(l)} = [m_{i1}^{(l)}, ..., m_{ik}^{(l)}]$, $m_i^{(l)} \in \mathbb{R}^{k \times d_h}$.

4.2 Neighbor Attention Layer

For our $l$-th attention layer with both self and neighbor attentions, we have inputs of neighbor representations $m_i^{(l)} = [m_{i1}^{(l)}, ..., m_{ik}^{(l)}]$, and hidden representations $h_i^{(l)} = [h_1^{(l)}, ..., h_n^{(l)}]$. Output of the self-attention is:

$$h_s^{(l)} = f(MHA(Q(h_i^{(l)}), K(h_i^{(l)}), V(h_i^{(l)}))),$$

where MHA is the standard multhead self-attention function (Appendix C), $f$ denotes the linear transformation function, $Q$, $K$, $V$ denote the query, and key-value pairs. All parameters above are fixed from a pretrained model.

We then apply attention across inputs and their corresponding neighbors. At the $i$-th position, representations considered for neighbour attention are $h_i^{(l)}$ and $m_i^{(l)}$. To avoid deviating too far from the pretrained model, we do not backpropagate gradients through $h_i^{(l)}$ during training. To get neighbor attentions, we train new key-value functions $K_b$, and $Q_b$. Representations after neighbor attention

Figure 2: The attention layer with both self and neighborhood attentions. The left side shows how we combine representations of neighbor and self attentions. After combination, the neighbor representations on the $l$-th layer will be considered in self attentions on the $(l + 1)$-th layer. The right side shows the attention layer with both self and neighbor attentions. Tokens / neighbors in one dashed box are considered when calculating self/neighbor attentions. The key and value functions are trained for neighbor attentions.

4 Transformer with Neighbor Attentions

Our neighbor attention model is based on a frozen pretrained model with neighbor attentions added to specific layers to help establish connections among label and sentence tokens. Section 4.1 introduces the selection of neighbors of each token, and 4.2 describes the details of the neighbor attention layer.

4.1 Neighbor Selection

The token embedding layer, which contains embeddings $e$ of all tokens from the vocabulary, can be used to get neighbors of each token. Denote the $n$ input token representations on the $l$-th layer as $h^{(l)} = [h_1^{(l)}, ..., h_n^{(l)}]$. After propagations over several layers, we still observe strong correlation between $h_i^{(l)}$ and $e$ at different layers of BERT-base (Appendix B), which may due to the residual connections (He et al., 2016) at each layer. In this case, we calculate similarities among the $i$-th input representation and token embeddings by:

$$\text{Sim}(e, h_i^{(l)}) = \exp(W_e(h_i^{(l)})^T / \sqrt{d_h}),$$

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where $d_h$ represents the dim of representations, $h_i^{(l)} \in \mathbb{R}^{1 \times d_h}$, $W_e \in \mathbb{R}^{|V| \times d_h}$ is the matrix of a pretrained token embeddings, $|V|$ represents the vocabulary size. We then randomly select $k$ tokens out of $K$ candidates to be neighbors of $h_i^{(l)}$, where candidates are tokens with top-$K$ similarity scores of $h_i^{(l)}$. Here, $K$ controls the range of the initial neighborhood. In this work, we set $k = 10$, $K = 100$. The corresponding neighbor embeddings are extracted from the vocabulary $W_e$ with the $i$-th positional embedding added.

We then apply a transformation to transfer neighbor representations from $e$ space to $h$ space. For the $j$-th neighbor of $h_i^{(l)}$ with embedding $e_{ij}$, the new representation $m_{ij}^{(l)}$ is:

$$m_{ij}^{(l)} = \text{LN}_e(f_e(e_{ij} - e_i) + (e_{ij} - e_i) + h_i^{(l)}),$$

where $e_i$ is the embedding of the $i$-th input, $f_e$ is a linear function: $\mathbb{R}^{d_h} \rightarrow \mathbb{R}^{d_h}$, ‘LN’ represents $Layer\;\text{Norm}$. Better choices for this transformation may further benefit the representation learning, which we leave for future studies. After this step, neighbor representations of $h_i^{(l)}$ are denoted as $m_i^{(l)} = [m_{i1}^{(l)}, ..., m_{ik}^{(l)}]$, $m_i^{(l)} \in \mathbb{R}^{k \times d_h}$.

4.2 Neighbor Attention Layer

For our $l$-th attention layer with both self and neighbor attentions, we have inputs of neighbor representations $m_i^{(l)} = [m_{i1}^{(l)}, ..., m_{ik}^{(l)}]$, and hidden representations $h_i^{(l)} = [h_1^{(l)}, ..., h_n^{(l)}]$. Output of the self-attention is:

$$h_s^{(l)} = f(MHA(Q(h_i^{(l)}), K(h_i^{(l)}), V(h_i^{(l)}))),$$

where MHA is the standard multhead self-attention function (Appendix C), $f$ denotes the linear transformation function, $Q$, $K$, $V$ denote the query, and key-value pairs. All parameters above are fixed from a pretrained model.

We then apply attention across inputs and their corresponding neighbors. At the $i$-th position, representations considered for neighbour attention are $h_i^{(l)}$ and $m_i^{(l)}$. To avoid deviating too far from the pretrained model, we do not backpropagate gradients through $h_i^{(l)}$ during training. To get neighbor attentions, we train new key-value functions $K_b$, and $Q_b$. Representations after neighbor attention
are \( h_b^{(l)} = [h_{b1}^{(l)}, ..., h_{bn}^{(l)}] \), with each \( h_{bi}^{(l)} \) as:
\[
h_{bi}^{(l)} = f(MHA(Q(h_{i}^{(l)}), K_{b}(r_{i}^{(l)}), V_{b}(r_{i}^{(l)})))
\]
\[
r_{i}^{(l)} = [sg(h_{i}^{(l)}), m_{i1}^{(l)}, ..., m_{ik}^{(l)}]
\]
where ‘\( sg \)’ represents ‘stop gradient’, \( K_{b}, V_{b} \) denote the learnable key and value functions for neighbor attentions. Representations from self and neighbor attentions are then combined as hidden representations of the next layer:
\[
h^{(l+1)} = LN((1 - \alpha)h_i^{(l)} + \alpha h_{b}^{(l)} + h_l^{(l)}),
\]
where \( LN \) represents the LayerNorm given from the pretrained model, and \( \alpha \) is a pre-defined scalar weight, which we set as 0.1 in our case.

The neighbor representation \( m_i \) is also updated at each layer. Assuming each neighbor of \( h_i^{(l)} \) is influenced only by \( m_i^{(l)} \), \( h_i^{(l)} \) and \( h_{[\text{MASK}]}^{(l)} \), neighbor representations are updated by:
\[
m_i^{(l+1)} = LN(m_{i}^{(l)} + m_{i}^{(l)})
\]
\[
m_{i}^{(l)} = f(MHA(Q(m_{i}^{(l)}), K_{b}(z_{i}^{(l)}), V_{b}(z_{i}^{(l)})))
\]
\[
z_{i}^{(l)} = [sg(h_{i}^{(l)}), sg(h_{[\text{MASK}]}^{(l)}), m_{i1}^{(l)}, ..., m_{ik}^{(l)}]
\]

A figure of the attention layer with both neighbor and self attentions is shown in Fig. 2. Adding neighbor attentions on more layers will increase the reachability of the propagation, but can also result in over-smoothing (Shi et al., 2022), e.g. neighbor tokens all have similar representations regardless of semantics. In this work, we add neighbor attentions to at most the last half of the transformer layers in the pretrained model. To be regularized by self-attention, we always leave the last layer weights frozen (as pretrained self-attention weights).

## 5 Regularization

One advantage of the neighbor attention model is that neighborhood representations correspond directly to input tokens, which makes it easier to guide the training of those representations, compared to prompt tuning. To better learn the sentence representation, we introduce two regularizations.

**Expressiveness Regularization**  In our problem, the \([\text{MASK}]\) representation should be expressive enough to allow inference of both the context and label tokens. To encourage expressiveness, we guide \( h_{[\text{MASK}]} \) at each layer to be close to neighbors of context and label tokens, as measured by cosine similarity:
\[
L_{m}^{(l)} = \mathbb{E}_{i \in \{x_1, x_2, x'_y\}} \mathbb{E}_{j} \text{cos}(h_{[\text{MASK}]}^{(l)}, sg(m_{ij}^{(l)})).
\]
We estimate the expectation on neighbors by uniformly sampling a neighbor from the \( k \) neighbors at each time when calculating the cosine similarity.

**Neighborhood Regularization**  Since \( L_{m} \) above is directly related to neighbor representations, we add a regularization to discourage neighbor representations moving too far away from context representations. The regularization term is:
\[
L_{n}^{(l)} = \mathbb{E}_{ij} \text{cos}(sg(h_{i}^{(l)}), m_{ij}^{(l)}).
\]
This encourages each neighborhood to stay near its context representation, and not easily migrate to arbitrary spaces. The objective with regularizations is then to maximize Eq. (2) + \( E_l[L_{m}^{(l)}] + E_l[L_{n}^{(l)}] \).

**Connecting Tokens**  The capacity of our model depends highly on the mobility of neighbor representations, which allows for connections to related tokens. However, with regularization \( L_{m} \), the mobility of neighborhood is limited. To increase model capacity, we add additional \([\text{MASK}]\) tokens (denoted as \([\text{MASK}]'\)) at the beginning of each segment as below:
\[
[\text{CLS}] [\text{MASK}]' \{Y\} [\text{MASK}] [\text{SEP}] [\text{MASK}]' x_1 [\text{SEP}] [\text{MASK}]' x_2 [\text{SEP}]. (4)
\]
The extra \([\text{MASK}]\) tokens increase connectivity between other tokens, allowing for more neighborhood propagation. Details of the selection of connecting tokens are discussed in Appendix D.

## 6 Experiments

Our experiments assess the influence of the task formulations we introduce, the trade-off between expressiveness and classification, and the impact of regularization strategies.

### 6.1 Tasks and Metrics

**Target Tasks**  We report classification performance on five target tasks from the GLUE benchmark (Wang et al., 2019), where the semantics of the classes can be clearly specified via simple label tokens: text entailment tasks (RTE, MNLI) (Williams et al., 2018); question entailment task
We compare against standard fine-tuning, prompt-based models, and other parameter efficient models to see the effects of different model structures and parameter numbers. For all models, we use BERT-base as the pretrained model. We compare the following models: (1) **NeighAttn**: our neighbor attention model, with or without regularizations. (2) **Fine-tuning (FT)**: fully fine-tuned models. (3) **Prompt Tuning (ProT)** (Lester et al., 2021): tuning embeddings of prompt tokens added in inputs for target tasks. The prompt length is 100. (4) **Prefix Tuning v2 (PT2)** (Liu et al., 2021b): tuning different embeddings added in inputs of each attention layer. We set 50 as prompt length and apply layer normalization on added embeddings at each layer to accelerate training. (5) **Adapter** (Houlsby et al., 2019): a parameter efficient model with adapters injected after attention blocks at each layer. (6) **BitFit** (Zaken et al., 2021): bias-only tuning based on the frozen pretrained model.

All models are implemented in Pytorch (Paszke et al., 2019), with tokenizers imported from the Huggingface package (Wolf et al., 2020). For NeighAttn models, we train with learning rates selected from \{2e-4, 5e-4, 1e-3\} and \{5, 8\} epochs. We add neighbor attentions on the 7-th to 11-th layers of the transformer. For prompt-based models, prompt lengths are selected according to settings in source papers, training with \{10, 20, 50\} epochs.

### 6.3 Results

#### Influence of the Task Formulation

We compare the influence of the different task formulations on 10% SNLI data in Table 1. Results show that training to predict from [CLS] representations may achieve high classification performance, but fare poorly in terms of expressiveness. However, training to predict from [MASK] tokens generates more expressive representations that can indicate reasonable rationales, while maintaining comparable classification scores. And by comparing input formats with and without label semantics (middle and lower blocks in table), we see consistent gains in both PT2 and NeiAttn’s expressiveness scores, which suggests that inputs with label tokens help to better connect label and sentence semantics resulting in better task-related information in the representation. Table 2 shows examples of top-10 [MASK] decodings for specific tasks.

| Recall@20 | Precision@1 | Accuracy |
|-----------|-------------|----------|
| [CLS]→y  | 5.8 (*)     | 85.8(*)  |
| PT2→y    | 2.0         | 85.1(*)  |
| NeiAttn→y| 8.5 (*)     | 84.8(*)  |

| Recall@20 | Precision@1 | Accuracy |
|-----------|-------------|----------|
| [CLS]→y  | 12.1 (*)    | 86.1(*)  |
| PT2→y    | 38.4(*)     | 84.9(*)  |
| NeiAttn→y| 38.2(*)     | 84.7(*)  |

| Recall@20 | Precision@1 | Accuracy |
|-----------|-------------|----------|
| [CLS]→y  | 13.0(*)     | 86.7(*)  |
| PT2→y    | 37.8(*)     | 85.1(*)  |
| NeiAttn→y| 36.3(*)     | 84.6(*)  |

Table 1: Model performance with different task formulations on 10% SNLI data. Precision@1 calculates the rate of the top-1 decoding that in keywords. \("(*)\) indicates the best score of each type of model.

#### Expressiveness vs. Classification Ability

We then compare different models with our task formulation in Eq. (1) and the objective in Eq. (2) in Table 3 and Table 4. Although fine-tuning achieves the best classification performance, it fares the worst in terms of expressiveness. This may be in part due to the loss of guidance of the pretrained knowledge on semantic correlations. Classification scores of the other models with frozen pretrained
Table 2: Examples of top-10 [MASK] decodings on SNLI (SN), QNLI (QN) and SST (SS) dataset. ‘NeiReg’ represents NeiAttn+reg. ‘kwd’ shows keywords given in e-SNLI for evaluation only.

| SN | s1  | Two women are embracing while holding to go packages. |
|    | s2  | The sisters are hugging goodbye while holding to go packages after just eating lunch. |
| Y  |     | Neutral |
| kwd | The sisters hugging goodbye after just eating lunch |
| PT2 | lunch dinner eating breakfast friends leaving food pizza reunion eat |
| NeiReg | goodbye farewell sister hugged new family hug reunion sad old |
| QN | s1  | What came into force after the new constitution was herald? |
| s2  | As of that day, the new constitution heralding the Second Republic came into force. |
| Y  | Entailment |
| NeiReg | , " first the and after of day it - |
| SS | s  | it ‘ s a charming and often affecting journey. |
| Y  | Positive |
| NeiReg | truly beautifully inspiring , and “ travel wonderful enjoyed unique |
|          | inspiring unique and wonderful entertaining enjoyable engaging beautiful charming very |

parameters are generally worse than FT; this suggests training with [MASK] tokens for target tasks is likely harder than with [CLS] tokens and may require more modeling capacity.

For the rest of our discussion on different training data sizes and target tasks, we focus only on the non-fine-tuning models. Table 3 compares classification and expressiveness results over different data volume regimes on the SNLI dataset. For classification, Adapter achieves the best scores on 3/4 sets, while PT2 and NeiAttn (+reg) also achieve comparable scores (<-1% to Adapter). Prompt tuning, which is known to be effective on large scale, is ineffective with the smaller base model. Interestingly, we find that better classification performance does not always correspond to better expressiveness. With more training steps, even when there is more data, the expressiveness scores of models like Adapter, PT2 and NeiAttn tend to decrease. The structure of models also leads to different expressiveness abilities. Compared to Adapter, PT2 and NeiAttn (+reg) can achieve much higher (>20%) expressiveness scores. Prompt tuning (ProT) also achieves consistently high expressiveness scores across sets. These observations show that introducing new ‘nodes’ (prompts, neighbors) can help models to better connect label and sentence semantics, thus nudging them closer towards predicting from rationales.

Table 4 compares models’ performance when training on different target tasks. The classification performance is measured on the target task dev sets but the expressiveness performance is measured by applying the model on the e-SNLI dev set. We use this as a generalization measure of expressiveness. NeiAttn (+reg) achieves the best classification scores on 2/5 tasks. For expressiveness, we have two main findings: First, bad classification ability will sometimes harm the expressiveness. For example, ProT has high expressivity scores but low classification scores on SNLI. However, for relatively difficult tasks like RTE, both classification and expressiveness scores are generally low. This raises an interesting question for further research on how to improve both aspects simultaneously. Second, overfitting harms expressiveness. We observe that models with a large gap in classification performance between training and dev sets of a task are likely to have low expressiveness scores on that task. And overfitting to biased reasoning will result in bad expressiveness. One manifestation of such overfitting can be seen when the top-10 decoded tokens from [MASK] often include punctuation marks; see the QNLI example in Table 2. Models with more parameters are more likely to suffer from such overfitting issue, and thus adding regularizations may help.

In general, PT2 and NeiAttn (+reg) achieve the best balance between classification and expressiveness, while NeiAttn (+reg) has the best expressiveness on 3/4 SNLI sets and 2/5 GLUE sets, with classification scores comparable to the best.

Impact of Regularization on the Model Models can overfit to biased reasoning for their decisions. In Table 2, PT2 has several punctuations in [MASK]’s top-10 decodings, which suggests it may rely on punctuations to connect among label and sentence semantics. In our neighbor attention model, adding regularization on neighbor representations can mitigate such biased reasoning. With regularization, NeiAttn+reg achieves significant improvement (~5%) in expressiveness on SNLI data and ~3% improvement on RTE, as shown in Table 3 and Table 4. Compared to PT2, which contains punctuations in the SST example (Table 2), NeiAttn+reg’s top-10 decoding contains more tokens close to rationales. However, adding specific
Table 3: Classification and expressiveness performance on different ratios of SNLI dataset. **Bold face** are the best scores in non-fine-tuning (FT) methods, **underline** scores are the second best. ‘Recall’ means the Recall@20.

| Method    | SNLI (549k) | 1% Acc  | 10% Acc | 30% Acc | 50% Acc | 1% Recall | 10% Recall | 30% Recall | 50% Recall |
|-----------|-------------|---------|---------|---------|---------|-----------|------------|------------|------------|
| FT        | 79.4        | 19.7    | 86.0    | 12.1    | 88.7    | 12.6      | 90.0       | 10.9       |
| Adapter   | **79.0**    | 21.0    | **85.4**| 13.5    | **87.9**| 7.2       | **89.2**   | 6.1        |
| BitFit    | 78.7        | 38.4    | **85.5**| 34.4    | 86.3    | 35.5      | 87.5       | 35.5       |
| ProT      | 73.7        | 43.2    | 82.4    | **44.2**| 84.6    | 40.4      | 85.1       | 38.2       |
| PT2       | 78.7        | 39.5    | 84.9    | 38.4    | 87.2    | 36.2      | 88.4       | 36.4       |
| NeiAttn   | 78.9        | 41.4    | 84.7    | 38.2    | 87.3    | 36.1      | 88.0       | 32.2       |
| NeiAttn+reg | 78.6       | **45.6**| 85.0    | 43.5    | **87.1**| **42.0**  | 88.0       | **40.5**   |

Table 4: Classification and expressiveness performance on selected GLUE datasets. **Bold face** are the best scores in non-fine-tuning (FT) methods, **underline** scores are the second best. ‘Recall’ means the Recall@20.

| %params | RTE (2.5k) | SST-2 (67k) | QNLI (105k) | QQP (364k) | MNLI-m (393k) |
|---------|------------|-------------|--------------|------------|---------------|
|         | Acc        | Recall      | Acc          | Recall      | Acc            |
| FT      | 100%       | 67.1        | 7.7          | 91.6        | 8.5            |
| Adapter | 2.3%       | 65.3        | 17.4         | 90.7        | 16.5           |
| BitFit  | 0.5%       | 66.1        | 27.7         | 90.4        | 20.7           |
| ProT    | 0.5%       | 60.3        | 13.4         | 86.9        | 10.0           |
| PT2     | 0.8%       | 66.4        | 42.1         | **91.4**    | 30.2           |
| NeiAttn | 5.4%       | **67.1**    | **41.4**     | 90.7        | **35.1**       |
| NeiAttn+reg | 5.4% | 66.1 | **44.2** | 90.6 | 31.4 | 90.0 | 20.7 | **88.7** | 23.2 | **81.6** | 35.5 |

regularization may negatively affect the generalization of the representations. When trained for the SST, QQP and MNLI tasks, the generalization of NeiAttn+reg’s expressiveness measured on e-SNLI drops. This may be because the decisions for different tasks require different reasoning patterns, which suggests the need for an expressiveness regularization that works across different tasks.

7 Related Work

**Prompt Tuning** Recently, GPT-3 is developed as a powerful few-shot learner with prompt design (prompting) (Brown et al., 2020). Compared to discrete prompting (Schick and Schütze, 2020; Shin et al., 2020), prompt tuning (Li and Liang, 2021; Lester et al., 2021; Liu et al., 2021c) is a method learning continuous prompts via backpropagation based on a frozen language model. Our method is in spirit similar to prompt tuning, but aims to learn the representation that can summarize task-related information in the input sentences.

**Parameter Efficient Tuning** Parameter efficient tuning learns for target tasks by tuning limited trainable parameters constructed on a pretrained model. Different methods include adding parameters at each transformer layer (Houlsby et al., 2019; Pfeiffer et al., 2021; He et al., 2021; Hu et al., 2021); or masking away existed parameters during training (Radiya-Dixit and Wang, 2020; Zaken et al., 2021). Based on a frozen pretrained model, our model also has the parameter efficient effect. However, since learning expressive representations requires sufficient model capacity, pursuing the parameter efficiency is not our main direction. Also, we build the model based on the learning of neighborhood representations, while remaining the body of the pretrained model untouched.

8 Conclusion

Learning expressive sentence representations can be beneficial in multiple respects including nudging the models to focus on true reasoning for the target task, understanding model behavior, and enabling better comparisons among samples in settings like contrastive learning. However, standard fine-tuning of [CLS] tokens turns out to be inadequate for expressiveness, while prompt tuning methods can be hard to control. To address this, we introduce a new task formulation that uses [MASK] tokens for numerical label prediction with label token space explicitly pointed out in the input. Further, we use a new neighbor-based attention method that can be regularized for connecting label and task-related sentence semantics. Our method is in spirit similar to prompt tuning, but with regularization we find it yields representations that achieve a better balance between classification performance and expressiveness without extra training for rationales.
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A Convex Hull in Fig. 1

In transformer models, the single-head self attention output of a layer can be expressed as

\[ h_i' = \sum_{j=1}^{n} \lambda_i^j f_u(h_j), \]

with \( \lambda_i^j \geq 0 \) and \( \sum_j \lambda_i^j = 1 \). Here \( \{h_0, ..., h_n\} \) are input representations, \( \{h_0', ..., h_n'\} \) are output representations, \( f_u \) is a linear function, and \( \lambda_i^j \) is the attention weight measuring the attention of \( h_j \) on \( h_i \). Imposing \( \lambda_i^j \geq 0 \) and \( \sum_j \lambda_i^j = 1 \) by the softmax function means that each output representation \( h_i' \) is within the convex hull of a linear transformation of input representations (Rockafellar, 2015). Since feed-forward functions added on the self attention outputs afterwards are independent at each token representation, we only show representations of the self attention module in Fig. 1.

Since representations out of the self attention module are within the convex hull of the linear-transformed representations of input tokens, it can be sensitive to inputs. And adding more relevant tokens in inputs may help to establish a better searching space for representation learning.

B Correlation Between Token Encodings and Embeddings

After projections over several layers, we still observe strong correlation between \( h^{(1)} \) and e at different layers of BERT-base. In Table 5, by looking at tokens which have the nearest embeddings to the given representation encoded at different transformer layers, we can find that closely related token embeddings can be retrieved. However, after projections over several layers, the correlation among token embeddings and layer representations may be decreased. This may call for better neighbor selection strategies.

C Multi-head Self Attention

In conventional self-attention, we compute attention based on queries \( Q \in \mathbb{R}^{p \times d} \) and key-value pairs \( K \in \mathbb{R}^{g \times d}, V \in \mathbb{R}^{g \times d} \):

\[
\text{Attn}(Q, K, V) = \text{softmax}\left(\frac{QK^T}{\sqrt{d_h}}\right)V, \quad (5)
\]

where \( p, g \) are numbers of queries and key-value pairs. In multi-head attentions, we define the query, key, value functions of the \( i \)-th head as:

\[
Q_i(x) = xW_q^{(i)} \quad K_i(x) = xW_k^{(i)} \quad V_i(x) = xW_v^{(i)}
\]

where \( W_q^{(i)}, W_k^{(i)}, W_v^{(i)} \in \mathbb{R}^{d_h \times d} \) are projection matrices of queries, keys and values. \( x \) represents any input representation in \( \mathbb{R}^u \), \( u \) is the dimension varies with different \( x \). The output of the multi-head attention is the concatenation of outputs of all heads:

\[
\text{MHA}(Q(x), K(x), V(x)) = \text{cat}(\text{head}_1, \ldots, \text{head}_t)
\]

where \( t \) is the number of heads, and typically we have \( d_h = td \). The output is then projected by a linear \( f: \mathbb{R}^{d_h} \rightarrow \mathbb{R}^{d_f} \), and followed by the layer normalization (Ba et al., 2016) and residual connection to get the output of the layer.

D Impact of Connecting Tokens

In this paper, we use two kinds of connecting tokens: (1) ‘or’ in Eq. (1) to connect different label tokens; (2) ‘[MASK]’ in Eq. (4) to improve connectivity of neighborhoods under the regularization. The connecting tokens in different cases have to be selected carefully. In Section 6.3, we observe that connections leading to biased reasoning are usually established via punctuations. Punctuations are mostly used connecting tokens, and thus are highly connected to many tokens in the vocabulary, including ones unrelated to the sample.

In the first case, we use ‘or’ instead of punctuation (e.g. ‘.’) as the connecting token in Eq. (1) to avoid introducing extra connectivity through the input. In the second case, we use ‘[MASK]’ as the connecting token in Eq. (4) because it is
highly connected to many tokens but guided by the pre-trained model. In our model, with the help of the neighbor attention mechanism, we do not rely heavily on specific connecting tokens to make connections. And we only add very limited connecting tokens at the beginning of each segment. In practice, to further reduce the unnecessary reliance on specific connecting tokens (e.g. existed punctuations in sentence inputs), we randomly select 15% tokens in inputs which are not updated by the neighbor attention.

In general, we can utilize specific connecting tokens to accelerate the establishment of connections among label and sentence semantics. However, we should also control the reliance on these connecting tokens to reduce connections resulting in biased reasoning.

E Metrics

Denote the set of relevant keywords of the $i$-th sample as $\text{rel}_i$, the set of top-$k$ predicted words as $\text{pred}_{i}@k$. The two metrics used in this paper are:

- **Recall@k**, which calculates the proportion of keywords that are decoded in $\text{pred}_{i}@k$, is defined as:

  $$\text{Recall}@k = \mathbb{E}_i[|\text{pred}_{i}@k \cap \text{rel}_i|/|\text{rel}_i|].$$

- **Precision@k**, which calculates the proportion of tokens that decoded in $\text{pred}_{i}@k$ are keywords, is defined as:

  $$\text{Precision}@k = \mathbb{E}_i[|\text{pred}_{i}@k \cap \text{rel}_i|/k].$$

In Table 1, we use Precision@1 to evaluate whether the learned representations tend to contain interpretable task-related information from sentence inputs, and use Recall@20 to further evaluates the representations’ expressiveness ability.