## Improving word mover's distance by leveraging self-attention matrix

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#### Abstract

Measuring the semantic similarity between two sentences is still an important task. The word mover's distance (WMD) computes the similarity via the optimal alignment between the sets of word embeddings. However, WMD does not utilize word order, making it challenging to distinguish sentences with significant overlaps of similar words, even if they are semantically very different. Here, we attempt to improve WMD by incorporating the sentence structure represented by BERT's self-attention matrix (SAM). The proposed method is based on the Fused Gromov-Wasserstein distance, which simultaneously considers the similarity of the word embedding and the SAM for calculating the optimal transport between two sentences. Experiments demonstrate the proposed method enhances WMD and its variants in paraphrase identification with near-equivalent performance in semantic textual similarity. Our code is available at https://github.com/ymgw55/ WSMD.

## 1 Introduction

The task of measuring the semantic textual similarity (STS) of two sentences is essential for natural language processing with various applications (Cer et al., 2017). There are several methods for measuring STS, among which many methods using Optimal Transport (OT) distance have been proposed and have shown good performance (Kusner et al., 2015; Huang et al., 2016; Chen et al., 2019; Yokoi et al., 2020).

OT theory gives a method to measure the difference between two distributions by setting the transport cost of a unit mass and considering the allocation of the transported mass to minimize the total cost. This allocation is called optimal transport, and the total cost is called the OT distance.

A basic form of OT distance is the Wasserstein distance, which measures the similarity between sets using the distance between the elements in

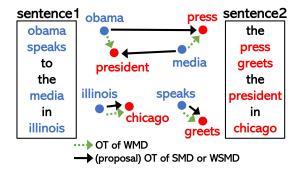


Figure 1: An illustration of OT for word embeddings from sentence 1 to sentence 2. Words are aligned by word similarity in WMD; e.g., *obama* matches *president*. Words are aligned by sentence structure in SMD or by word similarity and sentence structure simultaneously in WSMD; e.g., *obama* matches *press*. See Section 2.

the sets (Kantorovich, 1960). Word Mover's Distance (WMD) computes Wasserstein distance by considering a sentence as a set of word embeddings (Kusner et al., 2015).

However, WMD does not consider the word order of sentences, making it challenging to identify paraphrases. Let us see the following illustrative example of the paraphrases adapted from (Kusner et al., 2015) and (Zhang et al., 2019):

- (a) Obama speaks to the media in Illinois.
- (b) The President greets the press in Chicago.
- (c) The press greets the President in Chicago.

Here (b) is a paraphrase of (a), while (c) has a very different meaning from (a). However, all these sentences have a high overlap of words. Thus, WMD cannot distinguish these pairs.

To account for sentence structure, we focused on BERT (Devlin et al., 2019), an attention-based model that has recently achieved remarkable performance in natural language processing tasks. BERT is a masked language model that performs taskspecific fine-tuning after pre-training on a large

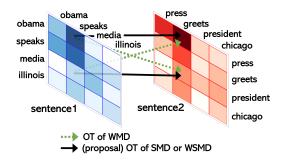


Figure 2: An illustration of OT for SAMs from sentence 1 to sentence 2. To avoid crowding the diagram, arrows are shown in only two SAM elements. The darker the color, the higher the value of the SAM element (reflecting a real SAM used in Table 1). The difference of SAM values is small for the word alignment of SMD or WSMD; e.g., (*obama, speaks*) matches (*press, greets*). The difference is large for that of WMD; e.g., (*obama, speaks*) matches (*president, greets*). See Section 2.

dataset. By inputting a sentence into the pretrained BERT, we can extract the Self-Attention Matrix (SAM), which represents the dependencies between words in the sentence. SAM encodes sentence structure information, such as syntactic information (Clark et al., 2019; Htut et al., 2019; Luo, 2021). Therefore, sentence structure can be incorporated into STS by measuring the distance between SAMs.

We propose a novel method called sentence Structure Mover's Distance (SMD) in Section 5 that measures the optimal transport distance between sentence structures represented in SAMs. SMD aims to find the optimal word alignment by considering the transport cost between elements of SAMs, while WMD considers the transport cost between word embeddings. To compute SMD, we employ the Gromov-Wasserstein (GW) distance (Mémoli, 2011; Peyré and Cuturi, 2020), the optimal transport distance for measuring structural similarity between sets.

SMD is ineffective by itself because it measures only the difference between sentence structures. Thus SMD is used in combination with WMD. We improve WMD-like methods (i.e., WMD and its variants based on Wasserstein distance between sets of word embeddings) by combining SMD with them in Section 6. This proposed method is called Word and sentence Structure Mover's Distance (WSMD). WSMD simultaneously measures the difference between word embeddings and the difference between sentence structures. WSMD employs the Fused Gromov-Wasserstein (FGW) distance (Vayer et al., 2019, 2020), known as the optimal transport distance that combines both Wasserstein and GW distances.

#### 2 Illustrative example

Here we explain how our proposed method works for the example of the paraphrases in Section 1. The original WMD and its improvement with our proposal are computed for this example and shown in Table 1. We computed these values using the word embeddings taken from the input layer of BERT and the SAMs taken from the second head of the eighth layer of BERT. The details of the setting will be described in Section 7.2. The similarity should be high for the sentence pair (a) vs. (b), i.e., case (1), while the similarity should be low for the sentence pair (a) vs. (c), i.e., case (2).

Looking at the values of the original WMD for the two cases, we find that they are about the same. Thus, WMD failed to give a reasonable sentence similarity. This failure is explained in Fig. 1 by illustrating word embeddings for case (2). WMD tries to find the closest word for each word, matching *obama* to *president*, *media* to *press*, and so on; the word alignment is indicated as the short dotted arrows. Then, WMD is computed by averaging the length of these short arrows, indicating a high sentence similarity contrary to the fact that the actual similarity is low for case (2).

However, the word alignment for WMD is inappropriate, given the word order and sentence structure. Our proposed method correctly matches *obama* to *press* and *media* to *president*. This word alignment is shown as the long arrows with solid lines in Fig. 1. WMD<sub> $\lambda$ </sub> in Table 1 is computed by averaging the length of these arrows, i.e., the same formula as WMD but using the OT taking account of the sentence structure. We find that WMD<sub> $\lambda$ </sub> increases for case (2), correctly indicating a low sentence similarity.

Fig. 2 explains how our proposed method takes account of the sentence structure. Given a word alignment between two sentences, we can think of a matching of elements between the two SAMs by applying the word alignment to both the rows and the columns of the matrices. For example, the word alignment of WMD in Fig. 1 induces the matching from (*obama*, *speaks*) to (*president*, *greets*), (*media*, *speaks*) to (*press*, *greets*), and so on. SMD minimizes the average difference of SAM values

case	sentences	WMD	$\mathrm{WMD}_{\lambda}$	WSMD	similarity
(1)	<ul><li>(a) obama speaks to the media in illinois.</li><li>(b) the president greets the press in chicago.</li></ul>	12.54	12.54	7.26	high
(2)	<ul><li>(a) obama speaks to the media in illinois.</li><li>(c) the press greets the president in chicago.</li></ul>	12.55	13.30	8.03	low

Table 1: Similarity measures for sentence pairs (a) vs. (b) and (a) vs. (c) of Section 1.

between the matched elements. This recovers the correct word alignment in this example. WSMD minimizes the weighted sum of the objectives for WMD and SMD; we used the mixing ratio  $\lambda = 0.5$  here. As shown in Table 1, WSMD correctly indicates that the sentences in case (2) are less similar than those in case (1).

## **3 Related Work**

This paper focuses on sentence similarity measures using the OT of word embeddings. For example, WMD (Kusner et al., 2015) uses uniform word weights and the  $L_2$  distance of word embeddings as the transport cost. By modifying the word weights and the transport cost, various WMD-like methods have been developed to compute sentence similarity based on the Wasserstein distance between sets of word embeddings. For example, Word Rotator's Distance (WRD) (Yokoi et al., 2020) uses the vector norm of the word embedding for the weight and the cosine similarity for the cost. There are many attempts to improve WMD by incorporating word order and sentence structure information into the weight, cost, and penalty terms, as explained below. However, none of them consider the optimal transport of sentence structures nor utilize SAMs from BERT.

In OPWD (Su and Hua, 2019), the temporal difference between word embeddings  $w_i$  and  $w'_j$  is measured by the distance between their relative temporal positions  $(i/n - j/m)^2$ , where *n* and *m* represent the lengths of the corresponding sentences. This difference is incorporated into the transport cost and an additional regularization term. WMDo (Chow et al., 2019) identifies consecutive words common to two sentences as a chunk and introduces a penalty term according to the number of chunks. In Syntax-aware WMD (SynWMD) (Wei et al., 2022), the word weight is computed from the word co-occurrence extracted from the syntactic parse tree of sentences, and a word embedding incorporates those from its subtree of the parse tree. The weight and the cost in SynWMD are called Syntax-aware Word Flow (SWF) and Syntax-aware Word Distance (SWD), respectively. In Recursive Optimal Transport Similarity (ROTS) (Wang et al., 2020, 2022), a recursive optimal transport method is introduced to capture word dependencies in sentences. To measure sentence similarity, the pairwise cosine similarity of words is weighted using this optimal transport and aggregated. In Mover-Score (Zhao et al., 2019), the inverse document frequency (IDF) is used for the word weight, and the word embeddings from BERT are used for computing the cost. BERTscore (Zhang et al., 2020a) also uses IDF and BERT embedding, but it employs greedy matching instead of OT for word alignment.

## 4 Optimal transport of words

We review the computation of WMD. In the following, we denote two sentences as

$$s = (\mathbf{w}_i)_{i=1}^n, s' = (\mathbf{w}'_j)_{j=1}^m \subset \mathbb{R}^d$$

where  $\mathbf{w}_i, \mathbf{w}'_j \in \mathbb{R}^d$  are word embeddings, and n, m are sentence lengths. SAM is denoted  $\mathbf{A} = (A_{ii'}) \in \mathbb{R}^{n \times n}$  and  $\mathbf{A}' = (A'_{jj'}) \in \mathbb{R}^{m \times m}$ , respectively, for *s* and *s'*. The element  $A_{ii'}$  is the attention weight from  $\mathbf{w}_i$  to  $\mathbf{w}_{i'}$ , and the element  $A'_{jj'}$  is the attention weight from  $\mathbf{w}'_j$  to  $\mathbf{w}'_{j'}$ . Each row of SAM is normalized as  $\sum_{i'=1}^n A_{ii'} = \sum_{j'=1}^m A'_{jj'} = 1$ .

The weights on  $\mathbf{w}_i$  and  $\mathbf{w}'_j$  in the probability distributions for s and s' are denoted by  $\mathbf{u} = (u_i)_{i=1}^n \in \mathbb{R}^n_{\geq 0}$ , with  $\sum_{i=1}^n u_i = 1$ , and  $\mathbf{u}' = (u'_j)_{j=1}^m \in \mathbb{R}^m_{\geq 0}$ , with  $\sum_{j=1}^m u'_j = 1$ , respectively. In this paper, unless otherwise stated, the weights on words in a sentence are equal, i.e., the uniform distribution specified as

$$\mathbf{u} = (1/n)_{i=1}^{n}, \, \mathbf{u}' = (1/m)_{i=1}^{m}.$$
 (1)

#### 4.1 Wasserstein distance

Sentences s and s' cannot be naively compared because they are generally different in length, and the corresponding words are unknown. We then consider the word transport from s to s' to obtain the word alignment. Interpret the sentence s as the amount of mass  $u_i$  at position  $\mathbf{w}_i$ . First, we denote  $P_{ij} \in [0, 1]$ , the amount of mass transported from position  $\mathbf{w}_i$  to position  $\mathbf{w}'_j$ , and consider the transport matrix  $\mathbf{P} = (P_{ij}) \in \mathbb{R}_{\geq 0}^{n \times m}$  with nonnegative elements. Next, we define the distance function  $c(\mathbf{w}_i, \mathbf{w}'_j) \in \mathbb{R}_{\geq 0}$  as the cost of transporting a unit mass from  $\mathbf{w}_i$  to  $\mathbf{w}'_j$  and specify the distance matrix  $\mathbf{C} = (C_{ij}) = (c(\mathbf{w}_i, \mathbf{w}'_j)) \in \mathbb{R}_{\geq 0}^{n \times m}$ . Given **P** and **C**, the transport from  $\mathbf{w}_i$  to  $\mathbf{w}'_j$  costs  $C_{ij}P_{ij}$ , and the total cost of transport is

$$\sum_{i=1}^{n} \sum_{j=1}^{m} C_{ij} P_{ij}.$$
 (2)

Finding the optimal transport matrix  $\hat{\mathbf{P}} = (\hat{P}_{ij})$  that minimizes the total cost, we compute the Wasserstein distance between s and s' as the minimum value of the total cost  $\sum_{i=1}^{n} \sum_{j=1}^{m} C_{ij} \hat{P}_{ij}$ .

#### 4.2 Word mover's distance

Word Mover's Distance (WMD) (Kusner et al., 2015) is Wasserstein distance applied to word embeddings. In the original WMD, the weight on words is the uniform distribution (1), and the distance function is Euclid distance between word embeddings  $\mathbf{w}_i$  and  $\mathbf{w}'_j$ . The distance matrix is defined as

$$C_{ij} = c(\mathbf{w}_i, \mathbf{w}'_j) = \|\mathbf{w}_i - \mathbf{w}'_j\|_2.$$
(3)

Therefore, WMD between s and s' is

$$WMD(s,s') = \min_{\mathbf{P}\in\mathbf{\Pi}(\mathbf{u},\mathbf{u}')} \sum_{i=1}^{n} \sum_{j=1}^{m} C_{ij} P_{ij}.$$
 (4)

Here,  $\Pi(u, u')$  is the set of all possible values of the transport matrix **P** defined as

$$\Big\{\mathbf{P}\in\mathbb{R}_{\geq 0}^{n\times m}\ \Big|\ \sum_{i=1}^n P_{ij}=u_j',\ \sum_{j=1}^m P_{ij}=u_i\Big\},\$$

and  $\mathbf{u}, \mathbf{u}'$  are omitted on the left side of (4).

#### 4.3 Limitations of WMD

WMD cannot account for the word order of the sentences because it treats a sentence as a set of word embeddings to find the optimal transport distance. Therefore, it is hard to distinguish sentence pairs with significant word overlaps in the case of static word embeddings. For some models, such as BERT and ELMo, the problem remains even for dynamic word embeddings that depend on the context because the similarity is still high between word embeddings of the same word (Ethayarajh,

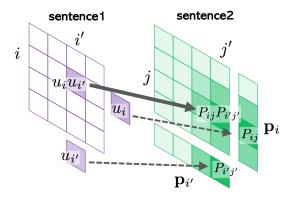


Figure 3: Transport of sentence structure induced by word transport. The array of transport from the *i*-th word is  $\mathbf{p}_i$  and that from the *i'*-th word is  $\mathbf{p}_{i'}$ . The amount of transport from the (i, i')-th element of SAM is defined by the outer product of  $\mathbf{p}_i$  and  $\mathbf{p}_{i'}$ .

2019). WMD does not distinguish the case (1) and the case (2) of Table 1 in Section 2 using the 0th layer of BERT as a statistic word embedding. Moreover, the difference is slight even if the 12th layer of BERT is used as a dynamic word embedding: WMD = 9.17 for case (1) and WMD = 9.26 for case (2).

# 5 Optimal transport of sentence structures

In this section, we propose to apply the GW distance to the SAM of BERT to measure the optimal transport distance between sentence structures. Later in Section 6, we will attempt to improve WMD using this method.

## 5.1 Gromov-Wasserstein distance

As seen in Section 2, the transport of sentence structure from s to s', i.e., transport from A to A', is induced by the transport of words. How can we define the structure transport consistent with a given word transport?

Let us consider  $\mathbf{p}_i = (P_{i1}, \dots, P_{im})$ , the array of transport amount  $P_{ij}$  from the *i*-th word of *s* to the *j*-th word of *s'*. As illustrated in Fig. 3, we apply  $\mathbf{p}_i$  to the *i*-th row of **A** and  $\mathbf{p}_{i'}$  to the *i'*-th column of **A**. This defines the transport from  $A_{ii'}$ of *s* to  $A'_{jj'}$  of *s'* as the outer product of  $\mathbf{p}_i$  and  $\mathbf{p}_{i'}$ ; the transport amount from position  $A_{ii'}$  to position  $A'_{jj'}$  is defined as  $P_{ij}P_{i'j'}$ .

The above definition of transport between SAMs is consistent with the transport of words. From the definition of transport, the mass at  $A_{ii'}$  is  $\sum_{j,j'=1}^{m} P_{ij}P_{i'j'} = u_iu_{i'}$ , and the mass at  $A_{jj'}$  is

 $\sum_{i,i'=1}^{n} P_{ij} P_{i'j'} = u'_{j} u'_{j'}$ . This implies that the marginal mass for rows and columns coincides with the mass of words, and thus the transport preserves the mass.

In this paper, we specify the cost of transporting a unit mass as  $|A_{ii'} - A'_{jj'}|^2$ . Then, the cost of transport is  $|A_{ii'} - A'_{jj'}|^2 P_{ij} P_{i'j'}$ , and the total cost of transport from **A** to **A**' is

$$\mathcal{E}_{\mathbf{A},\mathbf{A}'}(\mathbf{P}) := \sum_{i,i'=1}^{n} \sum_{j,j'=1}^{m} |A_{ii'} - A'_{jj'}|^2 P_{ij} P_{i'j'}$$
(5)

Finding the optimal transport matrix  $\hat{\mathbf{P}}$  that minimizes the total cost  $\mathcal{E}_{\mathbf{A},\mathbf{A}'}(\mathbf{P})$ , we compute the Gromov-Wasserstein (GW) distance (Mémoli, 2011; Peyré and Cuturi, 2020) between **A** and **A**' as the minimum value of (5).

#### 5.2 Sentence structure mover's distance

Applying the GW distance to SAMs, we propose the sentence Structure Mover's Distance (SMD), which is the optimal transport distance considering the dependency of words in a sentence.

$$SMD(\mathbf{A}, \mathbf{A}') = \min_{\mathbf{P} \in \mathbf{\Pi}(\mathbf{u}, \mathbf{u}')} \mathcal{E}_{\mathbf{A}, \mathbf{A}'}(\mathbf{P}) \quad (6)$$

Note that SMD is not a metric of a metric space, while it can still measure the structural difference. The general definition of GW distance considers the *p*-th root of the total cost for the form  $|A_{ii'} - A'_{jj'}|^p$  in (5), and it is a metric if  $A_{ii'}$  is a symmetric distance matrix. Thus using an asymmetric SAM is not GW distance in a strict sense. We consider the case p = 2 and the square root is omitted because it does not affect the magnitude order.

# 6 Optimal transport of words and sentence structures

Here, we propose an optimal transport distance that simultaneously considers the word embeddings and sentence structure.

# 6.1 Word and sentence structure mover's distance

As seen in Section 4.3, WMD computes Wasserstein distance using Euclid distance of word embeddings but cannot handle sentences with different meanings depending on word order. On the other hand, as seen in Section 5.2, SMD computes the GW distance using the SAM of BERT, which encodes the sentence structure, but it cannot handle individual word information like word embeddings. Therefore, by combining WMD-like methods (i.e., WMD and its variants obtained by modifying C, u and u') with SMD, we propose an optimal transport distance, Word and sentence Structure Mover's Distance (WSMD), that utilizes word features and considers word dependency within a sentence. By specifying the mixing ratio parameter  $\lambda \in [0, 1]$ , we obtain

WSMD((s, **A**), (s', **A**')) =  

$$\min_{\mathbf{P}\in\mathbf{\Pi}(\mathbf{u},\mathbf{u}')} \sum_{i,i'=1}^{n} \sum_{j,j'=1}^{m} \left\{ (1-\lambda)C_{ij} + \lambda k \left| A_{ii'} - A'_{jj'} \right|^2 \right\} P_{ij} P_{i'j'}, \quad (7)$$

where k is a normalization parameter. For further details about k, refer to Appendix A. By noting  $\sum_{i'=1}^{n} \sum_{j'=1}^{m} P_{i'j'} = 1$ , WSMD = WMD for  $\lambda = 0$ . For  $\lambda = 1$ , WSMD = kSMD.

For an intermediate value  $\lambda \in (0, 1)$ , WSMD considers both WMD and SMD. Let  $\hat{\mathbf{P}}$  be the optimal transport matrix, i.e.,  $\mathbf{P}$  that attains the minimum of (7). Substitute this  $\hat{\mathbf{P}}$  into (2) and (5), denote them as WMD<sub> $\lambda$ </sub> and SMD<sub> $\lambda$ </sub>, respectively. Then we can write

$$WSMD = (1 - \lambda)WMD_{\lambda} + \lambda kSMD_{\lambda}.$$
 (8)

This decomposition is explained in Appendix B.

The optimal transport distance that simultaneously considers the Wasserstein and GW distances, as in WSMD, is known as the Fused Gromov-Wasserstein (FGW) distance (Vayer et al., 2019, 2020). However, like SMD, WSMD uses an asymmetric SAM, so WSMD is not a metric in general.

## 7 Experiments

We compare the performance of our proposed method and existing baseline methods on the task of measuring semantic textual similarity (STS) between two sentences.

## 7.1 Datasets

## 7.1.1 PAWS dataset

Paraphrase Adversaries from Word Scrambling (PAWS) (Zhang et al., 2019) has a binary label for an English sentence pair indicating paraphrase (i.e., the sentence pair has the same meaning) or non-paraphrase. The binary classification of these labels can be considered an STS task. If the transport distance for a pair is small, we classify the pair as a paraphrase; otherwise, we classify it as a non-paraphrase. The effectiveness of this classification

	Dev	Test
PAWS <sub>QQP</sub>	1500 (24.7%)	677 (28.2%)
$PAWS_{Wiki}$	1500 (42.3%)	8000 (44.2%)
STSB	1500	1379

Table 2: The number of sentence pairs used in our experiments. Train sets are not used. The percentage of paraphrases for PAWS is shown in parentheses.

is then evaluated using the AUC as the metric.

There are two types of PAWS:  $PAWS_{QQP}$  and  $PAWS_{Wiki}$ , constructed from sentences in Quora and Wikipedia, respectively. Table 2 shows the number of sentence pairs and the percentage of paraphrases used in our experiments. In  $PAWS_{QQP}$ , since the test set is not provided, the first 1500 pairs were selected from the 11988 pairs in the train set to make a new dev set, and the original dev set was considered as a test set. In  $PAWS_{Wiki}$ , the first 1500 pairs were selected from the test set.

## 7.1.2 STS Benchmark dataset

The STSB dataset (Cer et al., 2017) contains human-annotated scores for English sentence pairs, reflecting the average similarity on a six-point scale. Table 2 shows the number of sentence pairs. Spearman's rank correlation (Spearman's  $\rho$ ) is used to compare these scores with optimal transport distances.

## 7.2 Models

We used BERT, SimCSE (Gao et al., 2021) and RoBERTa (Liu et al., 2020) from the Hugging Face transformers library (Wolf et al., 2020) and see Table 8 in Appendix C for details.

SimCSE is a sentence embedding model based on contrastive learning with BERT. It has two types: unsup-SimCSE and sup-SimCSE, depending on how positive samples are defined. In this study, unsup-SimCSE is used.

RoBERTa is a model that improves the performance of BERT by changing the pre-training settings of BERT, and by tuning the hyperparameters.

The BERT, SimCSE, and RoBERTa models we used have 12 layers and 12 heads, resulting in a total of 144 extractable SAMs. We input the sentences into BERT and removed the stopwords and special tokens such as [CLS] and [SEP] from the output tokens<sup>1</sup>.

The word embeddings used in the experiments are the static embeddings<sup>2</sup> taken from the input layer, i.e., the 0th layer, and the dynamic embeddings taken from the final layer, i.e., the 12th layer. We call such word embeddings BERT0, BERT12, and so on. When computing embeddings for STS methods such as WMD, recomputing the embeddings for each method may result in different embeddings due to the randomness of dropout. Therefore, to ensure an accurate comparison of STS methods, we had computed the embeddings once and used them for all the STS methods. We performed whitening for all the word embeddings because the representation of BERT is known to be anisotropic (Ethayarajh, 2019).

## 7.3 Baseline methods

The following simple baseline methods for representing a sentence were selected. The similarity for a sentence pair is computed by the cosine similarity of the two vectors.

**Bag-of-Words (BoW)** is a high-dimensional vector whose elements are the frequency of occurrence in a sentence for all words.

Average Pooling (Avg. Pool.) is simply the average vector of word embeddings in a sentence.

**[CLS] token**<sup>3</sup> is the first token in the input sequence, and in SimCSE it is used specifically for sentence embedding.

**SIF** (Arora et al., 2017) is an unsupervised method that sums word embeddings with frequency-based weights and subtracts the first singular vector from the SVD.

**uSIF** (Ethayarajh, 2018) is an unsupervised method that replaces the dot product with arccosine in the probability model of SIF and subtracts multiple singular vectors instead of just the first.

**Conceptor Negation (Con. Neg.)** (Liu et al., 2019) is an unsupervised method that optimizes the performance of sentence embeddings for a new corpus while preserving the performance for older corpora when dealing with multiple datasets.

**BERTScore** (Zhang et al., 2020b) is an automatic evaluation metric for text generation and computes a similarity score by comparing each token in a sentence with each token in another sen-

<sup>&</sup>lt;sup>1</sup>For one of the benchmarking OT methods (SynWMD),

we did not remove the stopwords since removing them would have deteriorated the performance.

<sup>&</sup>lt;sup>2</sup>Note that the embeddings taken from the 0th layer are only approximate statistic embeddings, because the segmentation embeddings and the position embeddings are added.

<sup>&</sup>lt;sup>3</sup>Instead of [CLS] token, we used <s> token for RoBERTa.

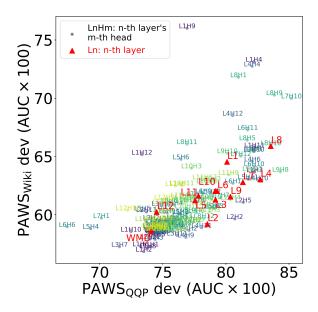


Figure 4: The AUC values of WMD ( $\star$ ) and WSMD ( $\bullet$ , **)** on the PAWS<sub>QQP</sub> (x-axis) and PAWS<sub>Wiki</sub> (y-axis) dev sets for BERT0. The  $\bullet$  symbol indicates the AUC value of the WSMD for a single head. The **\** symbol indicates the AUC value of the average WSMD for multi-heads within a layer. While there are significant variations in the  $\bullet$  symbols, the **\** symbols are more stable. In fact, the **\** symbols have a higher correlation coefficient than the  $\bullet$  symbols, as shown in Table 3.

WSMD calculation	#	$\rho \times 100$
single head $(\bullet)$	144	69.30
multi-heads within a layer ( $\blacktriangle$ )	12	74.50

Table 3: The Spearman's  $\rho$  between AUC values of WSMD for PAWS<sub>QQP</sub> and those for PAWS<sub>Wiki</sub> in Fig. 4. The average WSMD for multi-heads within a layer has a higher correlation than the WSMD for a single head.

tence.

**DynaMax** (Zhelezniak et al., 2019) is a fully unsupervised and non-parametric similarity that dynamically extracts and max-pools good features depending on the sentence pair.

#### 7.4 Benchmarking OT methods

The following OT methods computed from word embeddings were selected: WMD (Kusner et al., 2015) with the uniform and IDF weights. WRD (Yokoi et al., 2020) with the norm and IDF weights. SynWMD (Wei et al., 2022) with SWF weights and cost defined by cosine similarity and SWD. WMDo (Chow et al., 2019) with cost defined by cosine similarity. OPWD (Su and Hua,

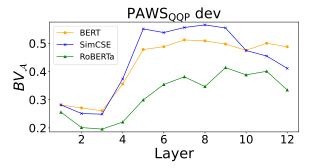


Figure 5: The layer-wise  $BV_A$  for BERT, SimCSE, and RoBERTa on the PAWS<sub>QQP</sub> dev set.  $BV_A$  is high from the fifth layer in each model.

	BERT	SimCSE	RoBERTa
Oth Embs.	8	6	9
12th Embs.	8	6	9

Table 4: Top1 layer for BERT, SimCSE, and RoBERTa. The layer was selected from the fifth onward based on the AUC of the average WSMD for a single layer using the  $PAWS_{QQP}$  dev set.

2019) with cost defined by  $L_2$  distance and cosine similarity. ROTS (Wang et al., 2020, 2022) using the most effective method ROTS+SWC+mean. We used Python Optimal Transport (POT) (Flamary et al., 2021) to implement simple WMD-like methods, SMD, and WSMD. We also used the OPWD part of the publicly available code for OWMD (Liu et al., 2018), but other parts could not be found.

#### 7.5 Head selection to compute SAM

Which heads should we use for WSMD? Fig. 4 shows the AUC values of WMD and WSMD for each head on the PAWS<sub>QQP</sub> and PAWS<sub>Wiki</sub> dev sets. It also shows the AUC values computed for the WSMD averaged over multiple heads within a layer. Table 3 shows the Spearman's  $\rho$  for AUC values in Fig. 4. These results suggest that when calculating WSMD, selecting an appropriate layer and using the average WSMD for multi-heads within that layer is likely to result in more stable performance than using a single head.

It is not desirable to change the heads or layers for each data set. Therefore, we first define *bidirectional attention variability*  $BV_A$  as a score for the layer containing SAMs that can capture the context of sentences. We then consider averaging WSMD using the SAMs of the layers selected based on  $BV_A$ . For details on  $BV_A$ , see Appendix E.

Fig. 5 shows the layer-wise  $BV_A$  for BERT, Sim-

SAM <sub>l</sub>	PAWS <sub>QQF</sub> AUC	$\begin{array}{c} \text{BERT0} \\ \text{PAWS}_{\text{Wik}} \\ \times 100 \end{array}$	$ \begin{bmatrix} \text{STSB} \\ \rho \times 100 \end{bmatrix} $	PAWS <sub>QQP</sub> AUC >	BERT12 PAWS <sub>Wik</sub> ( 100	$_{\rm i}$ STSB $\rho \times 100$
top 1	9.90	5.22	-0.74	0.26	0.66	-1.98
5-12	6.84	3.55	-0.53	-0.04	0.00	-1.32
1-12	7.38	3.32	-0.97	-0.06	-0.37	-1.34

Table 5: Average score improvement of WSMD for WMD-like methods with BERT.

SAMl	PAWS <sub>QQP</sub> AUC	$\begin{array}{l} \text{SimCSE0} \\ \text{PAWS}_{\text{Wiks}} \\ \times 100 \end{array}$	$ \begin{vmatrix} \text{STSB} \\ \rho \times 100 \end{vmatrix} $	S PAWS <sub>QQP</sub> AUC >		$r_{i}$ STSB $\rho \times 100$
top 1	5.44	1.67	-0.62	0.17	0.59	-0.93
5-12	4.39	0.90	-0.30	0.15	-0.06	-1.01
1-12	5.79	1.42	-0.73	0.33	-0.03	-1.20

Table 6: Average score improvement of WSMD for WMD-like methods with SimCSE.

$\mathrm{SAM}_l$	PAWS <sub>QQP</sub> AUC	RoBERTa0 PAWS <sub>Wiki</sub> × 100	$\left. \begin{array}{c} \text{STSB} \\ \rho \times 100 \end{array} \right $	Ro PAWS <sub>QQP</sub> AUC ×	BERTa12 PAWS <sub>Wik</sub> 100	$\stackrel{\rm i}{}_{\rho} \stackrel{\rm STSB}{\times 100}$
top 1	11.04	2.49	-0.74	0.01	0.37	-1.37
5-12	11.48	2.43	-0.88	0.13	0.24	-1.38
1-12	10.42	2.28	-1.10	-0.11	0.01	-1.41

Table 7: Average score improvement of WSMD forWMD-like methods with RoBERTa.

CSE, and RoBERTa on the  $PAWS_{QQP}$  dev set.  $BV_{\mathcal{A}}$  is high from the fifth layer in each model. Thus, we consider the following three ways to compute the average WSMD<sup>4</sup>: (i) The average WSMD using the best single layer from the fifth onward (top1 layer). (ii) The average WSMD over the fifth onwards (5-12 layers). (iii) The average WSMD over all the layers (1-12 layers). Table 4 presents the top1 layer chosen for each model. It is worth noting that the top1 layer selected using the PAWS<sub>QQP</sub> dev set was applied to all other datasets. It is also important to note that the selection of layers (i.e., 5-12 layers) in method (ii) was based only on  $\mathrm{BV}_\mathcal{A}$  of sentences from  $PAWS_{\mathrm{QQP}}$  dev set without any reference to the labels for the binary classification. In particular, method (iii) is fully unsupervised in terms of layer selection.

### 7.6 Results

Some WMD-like methods (WMD, WRD, Syn-WMD) are combined with SMD (as indicated as WSMD) and compared with the original method to see if an improvement by introducing WSMD. We use  $\lambda = 0.5$  for WSMD. For more details about the parameters for the other methods, see Appendix D.

WSMD is not attempted for ROTS, OPWD and WMDo because these methods cannot be expressed in the form (4).

#### 7.6.1 Comparison of WSMD Performance

Fig. 6 shows the experimental results compared to some baselines using BERT embeddings. For  $PAWS_{QQP}$  at the top of Fig. 6 and  $PAWS_{Wiki}$  at the middle of Fig. 6, the best-performing layer selection is the top1 layer, and improvements were observed in WSMD with WMD, WRD, and Syn-WRD for both BERT0 and BERT12. The top1 layer is chosen based on the  $PAWS_{QQP}$  dev set, therefore the performance improvement is greater in  $PAWS_{QQP}$  compared to  $PAWS_{Wiki}$ . For STSB at the bottom of Fig. 6, there is a small decrease in performance. However, especially with BERT0, performance can be improved on the PAWS datasets while still maintaining some level of performance on STSB.

Similar to Fig. 6, the experimental results for SimCSE and RoBERTa are shown in Appendix Figs. 7 and 8, respectively. We observe that the results are roughly similar to those for BERT, while the methods using RoBERTa0 show better performance compared to those using RoBERTa12 on STSB. Detailed results for each dataset are shown in Appendix Tables 19, 20, and 21.

#### 7.6.2 Comparison of layer selection methods

Tables 5, 6, and 7 show the performance improvement of WSMD using different head selection. It is observed that the performance on  $PAWS_{QQP}$ and  $PAWS_{Wiki}$  improves for all models when the top1 layer is selected. As shown in Fig. 6, particularly significant performance improvements are observed when the 0th-layer embeddings are used.

In addition, even for unsupervised layer selection, the performance improvements are seen on PAWS<sub>QQP</sub> and PAWS<sub>Wiki</sub> for all 0th-layer embeddings. In particular, for RoBERTa on PAWS, while the performance improves when using layers from 5 to 12 based on  $BV_A$ , the performance decreases when using layers from 1 to 12. This may suggest that the early layers do not have enough contextual information, as also indicated by BV<sub>A</sub> in Fig. 5.

For STSB, although no performance improvement is observed, the performance degradation is limited to a small 2%.

 $<sup>^4</sup>We$  used  $PAWS_{\rm QQP}$  dev set for the layer selection because it has better performance compared to  $PAWS_{\rm Wiki}$ , and also because STSB is a dataset with different properties than PAWS.

### 7.7 Supplementary experiments

In addition to the abovementioned experiments, we have conducted other experiments in different settings.

To evaluate the generality of our method, we conducted experiments with DistilBERT (Sanh et al., 2019) as a model with a different number of layers than BERT, and with BERT trained with a different seed (Sellam et al., 2022). We evaluated the performance of these models on  $PAWS_{QQP}$ ,  $PAWS_{Wiki}$ , and STSB. WSMD also showed strong performance on these models, especially on PAWS. More details can be found in Appendix G.

We also extended our experiments to another dataset, SICK-R (Marelli et al., 2014), using BERT to measure semantic textual similarity. Similar to STSB, the degradation in performance was within 2%. Detailed results of this additional study are also available in Appendix H.

Given the small size of the  $PAWS_{QQP}$  test set, which contains only 677 sentence pairs, we also present the scores on the  $PAWS_{QQP}$  train set using our method for WMD in Appendix I. The result suggests that improvements in paraphrase identification by WSMD are observed even when the dataset size increases.

These results confirm the effectiveness of our method on different datasets, using different models with SAMs.

#### 8 Conclusion

Since WMD treats a sentence as a set of word embeddings and computes sentence similarity, it cannot consider the word order in the sentence. Therefore, we focused on the fact that the SAM of the input sentence obtained from the pre-trained BERT represents the relationship between words in the sentence and has information on the sentence structure. We proposed an optimal transport distance WSMD that improves existing WMD-like methods by using FGW distance that simultaneously measures the difference between word embeddings and the difference between sentence structures. We conducted experiments on paraphrase identification on PAWS and sentence similarity on STSB, confirming the proposed method boosts PAWS performance with minimal impact on STSB.

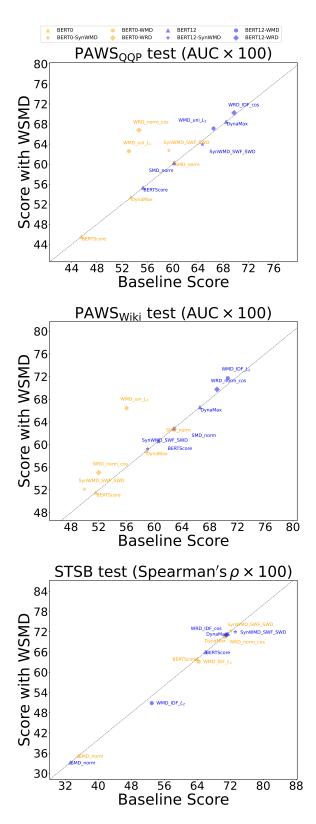


Figure 6: Performance of WSMD with several WMDlike methods (SMD, WMD, WRD, SynWMD) for BERT. The scores (AUC or Spearman's  $\rho$ ) are compared with the original WMD-like methods. Methods that are not applicable to WSMD are positioned on the diagonal line. Values above the diagonal line represent performance improvements achieved by WSMD.

## Limitations

- As seen in Section 7.6, there was not much improvement in scores on STSB compared to PAWS. Since methods like uSIF, which consider sentences as sets of words, show good performance, it is assumed that in STSB, unlike PAWS, there are fewer sentences where word order changes significantly alter the meaning, and the SMD term of WSMD is considered noise. In fact, in STSB, it was found that there is a strong correlation between the number of common words in a sentence pair and similarity. See the Appendix J for details.
- As noted in the Section 7.6, WSMD shows a smaller performance improvement with 12th embeddings compared to 0th embeddings in PAWS. This is probably due to the fact that the 12th embeddings are contextualized, and the changes in word order within sentences in PAWS are reflected in the embeddings.
- Sentences with the same meaning do not necessarily have the same structure. For example, *I don't think it makes sense* and *it doesn't make sense* are a pair of sentences with the same meaning. Still, they have different structures, so using WSMD might decrease the sentence similarity score.
- Compared to regular WMD, as the number of SAMs used in WSMD increases, the computation time also increases. However, since WSMD can be computed independently for each SAM, parallel processing is possible if resources are available.
- WSMD cannot be applied directly to other embeddings, such as word2vec, because different tokenizers are used for each embedding. However, it may be possible to use WSMD through processing such as replacing the tokens of the model with words in the other embeddings vocabulary.

## **Ethics Statement**

This study complies with the ACL Ethics Policy.

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### References

- Sanjeev Arora, Yingyu Liang, and Tengyu Ma. 2017. A simple but tough-to-beat baseline for sentence embeddings. In 5th International Conference on Learning Representations, ICLR 2017, Toulon, France, April 24-26, 2017, Conference Track Proceedings. Open-Review.net.
- Daniel M. Cer, Mona T. Diab, Eneko Agirre, Iñigo Lopez-Gazpio, and Lucia Specia. 2017. Semeval-2017 task 1: Semantic textual similarity multilingual and crosslingual focused evaluation. In *Proceedings* of the 11th International Workshop on Semantic Evaluation, SemEval@ACL 2017, Vancouver, Canada, August 3-4, 2017, pages 1–14. Association for Computational Linguistics.
- Liqun Chen, Yizhe Zhang, Ruiyi Zhang, Chenyang Tao, Zhe Gan, Haichao Zhang, Bai Li, Dinghan Shen, Changyou Chen, and Lawrence Carin. 2019. Improving sequence-to-sequence learning via optimal transport. In 7th International Conference on Learning Representations, ICLR 2019, New Orleans, LA, USA, May 6-9, 2019.
- Julian Chow, Lucia Specia, and Pranava Madhyastha. 2019. WMDO: fluency-based word mover's distance for machine translation evaluation. In *Proceedings* of the Fourth Conference on Machine Translation, WMT 2019, Florence, Italy, August 1-2, 2019 - Volume 2: Shared Task Papers, Day 1, pages 494–500. Association for Computational Linguistics.
- Kevin Clark, Urvashi Khandelwal, Omer Levy, and Christopher D. Manning. 2019. What does BERT look at? an analysis of bert's attention. In Proceedings of the 2019 ACL Workshop BlackboxNLP: Analyzing and Interpreting Neural Networks for NLP, BlackboxNLP@ACL 2019, Florence, Italy, August 1, 2019, pages 276–286. Association for Computational Linguistics.
- Jacob Devlin, Ming-Wei Chang, Kenton Lee, and Kristina Toutanova. 2019. BERT: pre-training of deep bidirectional transformers for language understanding. In Proceedings of the 2019 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies, NAACL-HLT 2019, Minneapolis, MN, USA, June 2-7, 2019, Volume 1 (Long and Short Papers), pages 4171–4186. Association for Computational Linguistics.
- Kawin Ethayarajh. 2018. Unsupervised random walk sentence embeddings: A strong but simple baseline. In Proceedings of The Third Workshop on Representation Learning for NLP, Rep4NLP@ACL 2018, Melbourne, Australia, July 20, 2018, pages 91–100. Association for Computational Linguistics.

- Kawin Ethayarajh. 2019. How contextual are contextualized word representations? comparing the geometry of bert, elmo, and GPT-2 embeddings. In Proceedings of the 2019 Conference on Empirical Methods in Natural Language Processing and the 9th International Joint Conference on Natural Language Processing, EMNLP-IJCNLP 2019, Hong Kong, China, November 3-7, 2019, pages 55–65. Association for Computational Linguistics.
- Rémi Flamary, Nicolas Courty, Alexandre Gramfort, Mokhtar Z. Alaya, Aurélie Boisbunon, Stanislas Chambon, Laetitia Chapel, Adrien Corenflos, Kilian Fatras, Nemo Fournier, Léo Gautheron, Nathalie T. H. Gayraud, Hicham Janati, Alain Rakotomamonjy, Ievgen Redko, Antoine Rolet, Antony Schutz, Vivien Seguy, Danica J. Sutherland, Romain Tavenard, Alexander Tong, and Titouan Vayer. 2021. POT: python optimal transport. J. Mach. Learn. Res., 22:78:1–78:8.
- Tianyu Gao, Xingcheng Yao, and Danqi Chen. 2021. Simcse: Simple contrastive learning of sentence embeddings. In Proceedings of the 2021 Conference on Empirical Methods in Natural Language Processing, EMNLP 2021, Virtual Event / Punta Cana, Dominican Republic, 7-11 November, 2021, pages 6894– 6910. Association for Computational Linguistics.
- Phu Mon Htut, Jason Phang, Shikha Bordia, and Samuel R. Bowman. 2019. Do attention heads in BERT track syntactic dependencies? In *Natural Language, Dialog and Speech (NDS) Symposium*. The New York Academy of Sciences.
- Gao Huang, Chuan Guo, Matt J. Kusner, Yu Sun, Fei Sha, and Kilian Q. Weinberger. 2016. Supervised word mover's distance. In Advances in Neural Information Processing Systems 29: Annual Conference on Neural Information Processing Systems 2016, December 5-10, 2016, Barcelona, Spain, pages 4862– 4870.
- Leonid Kantorovich. 1960. Mathematical methods of organizing and planning production. *Management Science*, 6(4):366–422.
- Matt J. Kusner, Yu Sun, Nicholas I. Kolkin, and Kilian Q. Weinberger. 2015. From word embeddings to document distances. In *Proceedings of the 32nd International Conference on Machine Learning, ICML* 2015, Lille, France, 6-11 July 2015, volume 37 of *Proceedings of Machine Learning Research*, pages 957–966. PMLR.
- Bang Liu, Ting Zhang, Fred X. Han, Di Niu, Kunfeng Lai, and Yu Xu. 2018. Matching natural language sentences with hierarchical sentence factorization. In Proceedings of the 2018 World Wide Web Conference on World Wide Web, WWW 2018, Lyon, France, April 23-27, 2018, pages 1237–1246. ACM.
- Tianlin Liu, Lyle Ungar, and João Sedoc. 2019. Continual learning for sentence representations using conceptors. In *Proceedings of the 2019 Conference of*

the North American Chapter of the Association for Computational Linguistics: Human Language Technologies, NAACL-HLT 2019, Minneapolis, MN, USA, June 2-7, 2019, Volume 1 (Long and Short Papers), pages 3274–3279. Association for Computational Linguistics.

- Yinhan Liu, Myle Ott, Naman Goyal, Jingfei Du, Mandar Joshi, Danqi Chen, Omer Levy, Mike Lewis, Luke Zettlemoyer, and Veselin Stoyanov. 2020. Roberta: A robustly optimized BERT pretraining approach. In 8th International Conference on Learning Representations, ICLR 2020, Addis Ababa, Ethiopia, April 26-30, 2020.
- Ziyang Luo. 2021. Have attention heads in BERT learned constituency grammar? In Proceedings of the 16th Conference of the European Chapter of the Association for Computational Linguistics: Student Research Workshop, EACL 2021, Online, April 19-23, 2021, pages 8–15. Association for Computational Linguistics.
- Marco Marelli, Luisa Bentivogli, Marco Baroni, Raffaella Bernardi, Stefano Menini, and Roberto Zamparelli. 2014. Semeval-2014 task 1: Evaluation of compositional distributional semantic models on full sentences through semantic relatedness and textual entailment. In *Proceedings of the 8th International Workshop on Semantic Evaluation, SemEval@COLING 2014, Dublin, Ireland, August 23-24, 2014*, pages 1–8. The Association for Computer Linguistics.
- Facundo Mémoli. 2011. Gromov-wasserstein distances and the metric approach to object matching. *Found. Comput. Math.*, 11(4):417–487.
- Gabriel Peyré and Marco Cuturi. 2020. Computational optimal transport.
- Alec Radford, Jeffrey Wu, Rewon Child, David Luan, Dario Amodei, and Ilya Sutskever. 2018. Language models are unsupervised multitask learners.
- Victor Sanh, Lysandre Debut, Julien Chaumond, and Thomas Wolf. 2019. DistilBERT, a distilled version of BERT: smaller, faster, cheaper and lighter. In 5th Workshop on Energy Efficient Machine Learning and Cognitive Computing @ NeurIPS 2019.
- Thibault Sellam, Steve Yadlowsky, Ian Tenney, Jason Wei, Naomi Saphra, Alexander D'Amour, Tal Linzen, Jasmijn Bastings, Iulia Raluca Turc, Jacob Eisenstein, Dipanjan Das, and Ellie Pavlick. 2022. The multiberts: BERT reproductions for robustness analysis. In The Tenth International Conference on Learning Representations, ICLR 2022, Virtual Event, April 25-29, 2022. OpenReview.net.
- Bing Su and Gang Hua. 2019. Order-preserving optimal transport for distances between sequences. *IEEE Trans. Pattern Anal. Mach. Intell.*, 41(12):2961– 2974.

- Titouan Vayer, Laetitia Chapel, Rémi Flamary, Romain Tavenard, and Nicolas Courty. 2020. Fused gromovwasserstein distance for structured objects. *Algorithms*, 13(9):212.
- Titouan Vayer, Nicolas Courty, Romain Tavenard, Laetitia Chapel, and Rémi Flamary. 2019. Optimal transport for structured data with application on graphs. In Proceedings of the 36th International Conference on Machine Learning, ICML 2019, 9-15 June 2019, Long Beach, California, USA, volume 97 of Proceedings of Machine Learning Research, pages 6275– 6284. PMLR.
- Jesse Vig and Yonatan Belinkov. 2019. Analyzing the structure of attention in a transformer language model. *CoRR*, abs/1906.04284.
- Zihao Wang, Jiaheng Dou, and Yong Zhang. 2022. Unsupervised sentence textual similarity with compositional phrase semantics. In *Proceedings of the 29th International Conference on Computational Linguistics, COLING 2022, Gyeongju, Republic of Korea, October 12-17, 2022,* pages 4976–4995. International Committee on Computational Linguistics.
- Zihao Wang, Yong Zhang, and Hao Wu. 2020. Structural-aware sentence similarity with recursive optimal transport. *CoRR*, abs/2002.00745.
- Chengwei Wei, Bin Wang, and C.-C. Jay Kuo. 2022. Synwmd: Syntax-aware word mover's distance for sentence similarity evaluation. *CoRR*, abs/2206.10029.
- Thomas Wolf, Lysandre Debut, Victor Sanh, Julien Chaumond, Clement Delangue, Anthony Moi, Pierric Cistac, Tim Rault, Rémi Louf, Morgan Funtowicz, Joe Davison, Sam Shleifer, Patrick von Platen, Clara Ma, Yacine Jernite, Julien Plu, Canwen Xu, Teven Le Scao, Sylvain Gugger, Mariama Drame, Quentin Lhoest, and Alexander M. Rush. 2020. Transformers: State-of-the-art natural language processing. In Proceedings of the 2020 Conference on Empirical Methods in Natural Language Processing: System Demonstrations, EMNLP 2020 - Demos, Online, November 16-20, 2020, pages 38–45. Association for Computational Linguistics.
- Sho Yokoi, Ryo Takahashi, Reina Akama, Jun Suzuki, and Kentaro Inui. 2020. Word rotator's distance. In Proceedings of the 2020 Conference on Empirical Methods in Natural Language Processing, EMNLP 2020, Online, November 16-20, 2020, pages 2944– 2960. Association for Computational Linguistics.
- Tianyi Zhang, Varsha Kishore, Felix Wu, Kilian Q. Weinberger, and Yoav Artzi. 2020a. Bertscore: Evaluating text generation with BERT. In 8th International Conference on Learning Representations, ICLR 2020, Addis Ababa, Ethiopia, April 26-30, 2020.
- Tianyi Zhang, Varsha Kishore, Felix Wu, Kilian Q. Weinberger, and Yoav Artzi. 2020b. Bertscore: Evaluating text generation with BERT. In 8th International Conference on Learning Representations,

ICLR 2020, Addis Ababa, Ethiopia, April 26-30, 2020. OpenReview.net.

- Yuan Zhang, Jason Baldridge, and Luheng He. 2019. PAWS: paraphrase adversaries from word scrambling. In Proceedings of the 2019 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies, NAACL-HLT 2019, Minneapolis, MN, USA, June 2-7, 2019, Volume 1 (Long and Short Papers), pages 1298– 1308. Association for Computational Linguistics.
- Wei Zhao, Maxime Peyrard, Fei Liu, Yang Gao, Christian M. Meyer, and Steffen Eger. 2019. Moverscore: Text generation evaluating with contextualized embeddings and earth mover distance. In Proceedings of the 2019 Conference on Empirical Methods in Natural Language Processing and the 9th International Joint Conference on Natural Language Processing, EMNLP-IJCNLP 2019, Hong Kong, China, November 3-7, 2019, pages 563–578. Association for Computational Linguistics.
- Vitalii Zhelezniak, Aleksandar Savkov, April Shen, Francesco Moramarco, Jack Flann, and Nils Y. Hammerla. 2019. Don't settle for average, go for the max: Fuzzy sets and max-pooled word vectors. In 7th International Conference on Learning Representations, ICLR 2019, New Orleans, LA, USA, May 6-9, 2019. OpenReview.net.

#### A WSMD definition details

For clarity, we rewrite equation (7). By specifying the mixing ratio parameter  $\lambda \in [0, 1]$ , we obtain

WSMD((s, **A**), (s', **A**')) =  

$$\min_{\mathbf{P}\in\mathbf{\Pi}(\mathbf{u},\mathbf{u}')} \sum_{i,i'=1}^{n} \sum_{j,j'=1}^{m} \left\{ (1-\lambda)C_{ij} + \lambda k \left| A_{ii'} - A'_{jj'} \right|^2 \right\} P_{ij} P_{i'j'}$$

where  $k = C_{\rm M}/A_{\rm MSE}$  is computed from

$$C_{\rm M} = \sum_{i=1}^{n} \sum_{j=1}^{m} \frac{C_{ij}}{nm}$$
$$A_{\rm MSE} = \sum_{i,i'=1}^{n} \sum_{j,j'=1}^{m} \frac{|A_{ii'} - A'_{jj'}|^2}{n^2 m^2}.$$

Note that our definition of k is only to increase the interpretability of  $\lambda$ , and k does not change the performance at all. By this definition,  $C_M$  represents the average of  $C_{ij}$ , and  $A_{MSE}$  the average of  $|A_{ii'} - A'_{jj'}|^2$ . From this, we can roughly consider  $C_{ij} \sim C_M$ ,  $|A_{ii'} - A'_{jj'}|^2 \sim A_{MSE}$ . If we employ k, then  $k|A_{ii'} - A'_{jj'}|^2 \sim C_M/A_{MSE} \cdot A_{MSE} \sim C_{ij}$ . With this formulation, we can use an easily interpretable value for  $\lambda$ , such as 0.5. By noting  $\sum_{i'=1}^{n} \sum_{j'=1}^{m} P_{i'j'} = 1$ , WSMD = WMD for  $\lambda = 0$ . For  $\lambda = 1$ , WSMD = kSMD. For an intermediate value  $\lambda \in (0, 1)$ , WSMD considers both WMD and SMD. We normalized  $\lambda$  by introducing the factor k in (7).  $C_M$  and  $A_{MSE}$  are interpreted as (2) and (5), respectively, by specifying  $P_{ij} = u_i u'_j$ with the uniform weight (1).

## B Decomposition of WSMD into WMD and SMD components

Let  $\hat{\mathbf{P}}$  be the optimal transport matrix of (7), i.e.,  $\mathbf{P}$  that attains the minimum of (7). Substitute this  $\hat{\mathbf{P}}$  into (2) and (5), denote them as WMD<sub> $\lambda$ </sub> and SMD<sub> $\lambda$ </sub>, respectively. Then we rewrite equation (8) as follows:

$$WSMD = (1 - \lambda)WMD_{\lambda} + \lambda kSMD_{\lambda}.$$

In case (2) of Table 1, we computed WSMD = 8.03, k = 688,  $\lambda = 0.5$ . This is decomposed into the components WMD<sub> $\lambda$ </sub> = 13.30 and kSMD<sub> $\lambda$ </sub> = 2.76. On the other hand, we can also compute WMD = 12.55 and kSMD = 2.76 in the same setting, which indicates that WSMD is not a simple interpolation of WMD and kSMD. This is because

the optimal transport matrices in the computation of WMD, SMD, and WSMD are all different in general, and in WSMD, the optimization considers the two components simultaneously.

Interestingly, the decomposition (8) indicates that  $WMD_{\lambda}$  can be interpreted as an improvement of WMD by utilizing  $(\lambda/(1 - \lambda))kSMD_{\lambda}$  as a penalty term. Thus, in addition to WSMD,  $WMD_{\lambda}$ can also be used as a sentence similarity measure, although this is not the main argument of this paper.

#### C Models

The Hugging Face models used in the experiments are presented in Table 8.

## **D** Parameters for each method

Parameters are shown for each method used in the experiments. We provide explanations for terms that may be unclear or less intuitive compared to the original notation in the paper. numSVToRemove means the number of singular vectors to be removed.

### D.1 SIF

Parameters of SIF used in the experiments are shown in Table 9.

#### D.2 uSIF

Parameters of uSIF used in the experiments are shown in Table 10.

#### **D.3** Conceptor Negation

Parameters of Conceptor Negation used in the experiments are shown in Table 11.

## D.4 ROTS

WE apply the most effective technique, ROTS+SWC+mean to ROTS. In this context, SWC+mean denotes a process that implements dimension-wise (S)caling (Ethayarajh, 2019), possesses SIF (W)eights, applies (C)onceptor Negation, and uses the *mean* in the aggregation of pair-wise cosine similarities of words. Parameters of ROTS used in the experiments are shown in Table 12.  $P_{reg}$  means prior regularization,  $C_{reg}$ means cosine regularization, and  $E_{reg}$  means entropy regularization. C also means interpolation coefficient. aggregation means how to handle different scores (*mean, max, min, last, no*).

model	Hugging Face model		
BERT	bert-base-uncased		
unsup-SimCSE	princeton-nlp/unsup-simcse-bert-base-uncased		
RoBERTa	roberta-base		
DistilBERT	distilbert-base-uncased		
$\text{BERT}_{\text{seed0}}$	google/multiberts-seed_0		

Table 8: Models of Hugging Face used in the experiments.

parameters	values	parameters	value
weight	SIF	weight	SIF
numSVToRemove	1	$\alpha_{CN}$	2

Table 9: Parameters of SIF used in the experiments.

parameters	values
weight	uSIF
numSVToRemove	5

Table 10: Parameters of uSIF used in the experiments.

## D.5 OPWD

Parameters of OPWD used in the experiments are shown in Table 13.

## D.6 WMDo

Parameter of ROTS WMDo in the experiments are shown in Table 14.

## D.7 SynWMD

Parameter of SynWMD used in the experiments are shown in Table 15.

Table 11: Parameters of Conceptor Negation used in the experiments.

parameters	values
weight	SIF
$lpha_{CN}$	2
numSVToRemove	1
parser	dependency tree
aggregation	mean
normed vectors	True
tree depth	5
$P_{reg}$	$\left[10, 10, 10, 10, 10\right]$
$C_{reg}$	0
$E_{reg}$	0
C	1

Table 12: Parameters of ROTS used in the experiments.

parameters	values
$\lambda_1$	10
$\lambda_2$	0.03
$\sigma$	10
Iteration	20

Table 13: Parameters of OPWD used in the experiments.

parameter	value
δ	0.2

Table 14: Parameter of WMDo used in the experiments.

parameter	value
a	1

Table 15: Parameter of SynWMD used in the experiments.

#### **E** Details of attention variability

We employ *attention variability* as proposed in (Vig and Belinkov, 2019). This measures the degree of attention variability across different inputs. A high variability implies that the attention head is contentdependent, while a low variability suggests that the head is content-independent. Mathematically, attention variability  $V_A$  is defined as:

$$V_{\mathcal{A}} = \frac{\sum_{x \in X} \sum_{i=1}^{|x|} \sum_{j=1}^{i} |A_{ij}(x) - \bar{A}_{ij}|}{2 \cdot \sum_{x \in X} \sum_{i=1}^{|x|} \sum_{j=1}^{i} A_{ij}(x)} \quad (9)$$

where  $\mathcal{A}$  represents the head contained in a given layer, x represents sentences of length |x| in the dataset X,  $\mathcal{A}(x) = (A_{ij}(x)) \in \mathbb{R}^{|x| \times |x|}$  is the specific SAM for each sentence x, and  $\overline{A}_{ij}$  is the average of  $A_{ij}(x)$  over all  $x \in X$ . V<sub> $\mathcal{A}$ </sub> is defined for GPT-2 (Radford et al., 2018), and the summation from 1 to *i* for *j* reflects the unidirectional structure of GPT-2.

We adapt the attention variability  $V_A$  to BERT by defining a *bidirectional attention variability*  $BV_A$  that measures the degree of attention variability across different inputs, where the summation for j ranges from 1 to |x|. It is defined as follows:

$$BV_{\mathcal{A}} = \frac{\sum_{x \in X} \sum_{i=1}^{|x|} \sum_{j=1}^{|x|} |A_{ij}(x) - \bar{A}_{ij}|}{2 \cdot \sum_{x \in X} \sum_{i=1}^{|x|} \sum_{j=1}^{|x|} A_{ij}(x)}$$
(10)

# F Detail results of experiments in Section 7

For PAWS<sub>QQP</sub>, PAWS<sub>Wiki</sub>, and STSB, the scores from BOWS, [CLS], uniform-weighted and IDFweighted SMD, methods that do not require word embeddings, are shown in Tables 16, 17, and 18, respectively. The scores for methods that depend on word embeddings are shown in Tables 19, 20, and 21. Similar to Fig. 6, the experimental results for SimCSE and RoBERTa are shown in Figs. 7 and 8.

methods	s layer weight	PAW BERT	S <sub>QQP</sub> (AU SimCSE	C × 100) RoBERTa
BOWS		44.56	44.56	46.16
[CLS]		60.24	62.39	57.76
SMD	top 1	59.84	59.70	60.95
	5-12 uniform	58.50	58.04	59.96
	1-12	56.23	58.35	57.27
	top 1	60.25	59.77	59.48
	5-12 IDF	57.99	59.30	57.19
	1-12	57.82	57.71	55.62

Table 16: The scores on the PAWS<sub>QQP</sub> test set for BOWS, [CLS], uniform-weighted and IDF-weighted SMD, methods that do not require word embeddings. Note that BERT and SimCSE have identical scores for BOWS because they use the same tokenizer.

methods	alayer weight	PAW BERT	S <sub>Wiki</sub> (AUC) SimCSE	C × 100) RoBERTa
BOWS [CLS]		48.86 57.94	48.86 58.02	50.59 56.29
SMD	top 1 5-12 uniform 1-12 top 1 5-12 IDF 1-12	$\begin{array}{r} 61.68\\ 62.98\\ 59.66\\ 62.73\\ 63.30\\ 60.83\end{array}$	58.51 60.91 58.82 59.22 59.92 58.96	58.18 58.69 57.18 53.86 53.08 51.89

Table 17: The scores on the PAWS<sub>Wiki</sub> test set for BOWS, [CLS], uniform-weighted and IDF-weighted SMD, methods that do not require word embeddings. Note that BERT and SimCSE have identical scores for BOWS because they use the same tokenizer.

methods	layer weig	ht STSB BERT	(Spearman' SimCSE	$s \rho \times 100)$ RoBERTa
BOWS [CLS]		68.82 41.17	68.82 75.23	67.93 40.75
SMD	top 1 5-12 unifo 1-12 top 1 5-12 IDI 1-12	30.48	17.51 35.41 33.78 19.48 39.18 37.65	23.21 27.71 27.50 26.11 31.47 31.76

Table 18: The scores on the STSB test set for BOWS, [CLS], uniform-weighted and IDF-weighted SMD, methods that do not require word embeddings. Note that BERT and SimCSE have identical scores for BOWS because they use the same tokenizer.

methods	layer	weight	cost	BERT0	BERT12	PAWS <sub>QQP</sub> ( SimCSE0	AUC × 100) SimCSE12	RoBERTa0	RoBERTa12	
Avg. Pool. BERTScore		uniform	-	52.96 45.52	64.33 54.78	50.96 45.41	63.00 51.74	45.46 41.91	63.04 51.61	
D 14		IDF		45.40	55.29	45.25	51.98	42.71	53.01	
DynaMax SIF				53.38 53.23	68.47 64.15	51.89 51.34	66.39 62.83	49.82 45.00	66.41 62.76	
uSIF				53.25	64.05	51.34	62.85	44.75	62.68	
Con. Neg.				53.05	64.17	51.21	63.04	44.85	62.83	
ROTS				53.07	64.71	56.48	65.00	47.38	64.50	
		1.0	$L_2$	53.07	66.48	53.01	65.58	48.35	66.69	
OPWD		uniform	cosine	54.30	69.98	54.41	67.38	48.40	68.81	
WMDo		uniform	cosine	43.86	56.33	43.71	50.33	44.25	61.49	
	top 1			60.31	60.19	58.40	58.08	59.97	58.74	
SMD	5-12	norm		58.55	56.89	57.78	56.16	59.27	57.44	
	1-12			58.35	56.55	57.55	56.34	57.39	56.08	
				53.07	66.48	53.01	65.58	48.35	66.69	
	top 1	2 uniform		62.58 ( <b>†</b> 9.51)	67.10 ( <b>↑</b> 0.62)	57.87 ( <b>† 4.86</b> )	65.85 ( <b>†</b> 0.27)	58.96 ( <u>† 10.61</u> )	66.74 ( <b>†</b> 0.05)	
	5-12			58.74 ( <b>†</b> 5.67)	66.77 ( <b>†</b> 0.29)	56.35 († 3.34)	65.94 ( <b>†</b> 0.36)	59.32 († 10.97)	66.95 ( <b>†</b> 0.26)	
WMD	1-12		- L <sub>2</sub>	59.41 ( <b>† 6.34</b> )	66.71 ( <b>†</b> 0.23)	57.54 ( <b>† 4.53</b> )	66.13 ( <b>†</b> 0.55)	58.33 ( <b>† 9.98</b> )	66.76 ( <u>↑</u> 0.07)	
				2	52.44	66.08	52.47	65.26	48.28	64.53
	top 1	IDF		61.54 ( <b>†</b> 9.10)	66.75 ( <b>†</b> 0.67)	56.72 (↑ 4.25)	65.58 ( <b>†</b> 0.32)	57.52 ( <b>†</b> 9.24)	$64.61 (\uparrow 0.08)$	
	5-12 1-12			57.90 ( <b>†</b> 5.46)	66.36 († 0.28) 66.31 († 0.23)	55.68 († 3.21) 56.83 († 4.36)	$65.66 (\uparrow 0.40)$	57.78 († 9.50) 56.80 († 8.52)	$64.65 (\uparrow 0.12)$	
	1-12			58.47 ( <b>† 6.03</b> )	00.31 (1 0.23)	50.85 (1 4.50)	65.80 ( <b>†</b> 0.54)	56.80 (° <mark>[* 8.52</mark> )	64.39 (↓ -0.14)	
				54.65	69.07	53.71	66.99	48.89	67.45	
	top 1	norm		66.80 († 12.15)	69.56 ( <b>† 0.49</b> )	60.38 ( <b>†</b> 6.67)	67.59 ( <b>† 0.60</b> )	60.87 († 11.98)	67.59 ( <b>†</b> 0.14)	
	5-12			63.84 ( <b>†</b> 9.19)	69.25 ( <b>↑</b> 0.18)	58.64 (↑ 4.93)	67.32 ( <b>†</b> 0.33)	62.34 († 13.45)	67.64 ( <b>†</b> 0.19)	
WRD	1-12		- cosine	64.62 ( <b>† 9.97</b> )	69.36 ( <b>†</b> 0.29)	60.84 (↑ 7.13)	<u>67.65</u> ( <b>† 0.66</b> )	61.18 († 12.29)	67.54 ( <b>†</b> 0.09)	
	4 1			53.94	69.73	54.01	67.07	48.88	66.12	
	top 1 5-12	IDF		$\frac{67.43}{64.77}$ ( $\uparrow$ 13.49)	$\frac{70.23}{(0.01)}$ ( $\uparrow$ 0.50)	62.09 ( <b>†</b> 8.08) 61.18 ( <b>†</b> 7.17)	$67.60 (\uparrow 0.53)$	60.06 († 11.18)	$66.25 (\uparrow 0.13)$	
	1-12			$65.47 (\uparrow 10.83)$	69.91 ( <b>↑</b> 0.18) 70.00 ( <b>↑</b> 0.27)	63.66 ( <b>†</b> 9.65)	67.40 († 0.33) 67.64 († 0.57)	60.71 († 11.83) 59.79 († 10.91)	66.23 (↑ 0.11) 66.15 (↑ 0.03)	
	1-12			N. 7	N 7				N	
				47.60	60.72	47.92	59.17	42.87	66.26	
	top 1		cosine	59.41 (↑ 11.81)	60.73 ( <b>↑</b> 0.01)	54.99 ( <b>†</b> 7.07)	58.89 ( <b>↓</b> -0.28)	59.73 († 16.86)	66.10 (↓ -0.16)	
	5-12			56.27 ( <b>†</b> 8.67)	60.37 (↓ -0.35)	54.78 ( <b>†</b> 6.86)	59.03 (↓ -0.14)	60.43 (↑ 17.56)	66.36 ( <b>†</b> 0.10)	
SynWMD	1-12	SWF		56.57 ( <u>† 8.97</u> )	60.26 (↓ -0.46)	55.82 ( <b>† 7.90</b> )	59.17 (-)	58.60 († 15.73)	65.80 (↓ - <b>0.46</b> )	
-	ton 1			59.41	64.71	58.47	62.47	57.85	$\frac{70.14}{1000}$	
	top 1		SWD	$62.74 (\uparrow 3.33)$	$63.95 (\downarrow -0.76)$	$60.15 (\uparrow 1.68)$	$62.03 (\downarrow -0.44)$	$\frac{64.20}{62.41}$ († 6.35)	69.97 (↓ -0.17) 70.11 (↓ 0.02)	
	5-12 1-12			60.63 († 1.22) 60.86 († 1.45)	$63.88 (\downarrow -0.83)$ $63.78 (\downarrow -0.93)$	59.27 ( <b>† 0.80</b> ) 59.65 ( <b>† 1.18</b> )	62.10 (↓ -0.37) 62.09 (↓ -0.38)	63.41 († 5.56) 62.94 († 5.09)	70.11 (↓ -0.03) 69.87 (↓ -0.27)	
	1-12			00.00 (  1.45)	05.76 (1 -0.95)	J9.05 (  1.16)	02.07 (1 -0.38)	02.74 (  3.09)	07.07 (1 -0.27)	

Table 19: The scores on the  $PAWS_{QQP}$  test set for the methods using the embeddings from BERT, SimCSE, and RoBERTa. For WMD, WRD, and SynWMD, the scores of WSMD and the original method are compared for each layer selection. Score increases are highlighted in red and score decreases are highlighted in blue. Maximum scores for each embedding are underlined.

methods	layer	weight	cost	BERT0	BERT12	PAWS <sub>Wiki</sub> (A SimCSE0	$AUC \times 100)$ SimCSE12	RoBERTa0	RoBERTa12
Avg. Pool. BERTScore		uniform	_	49.43 51.58	60.06 60.60	49.68 52.66	56.71 57.02	51.11 52.99	59.13 57.57
DynaMax SIF uSIF		IDF		51.58 58.88 49.31 49.29	60.60 66.60 59.90 60.03	52.73 51.99 49.62 49.59	56.92 62.37 56.70 56.75	52.03 53.87 51.09 51.13	55.79 65.05 59.23 59.27
Con. Neg. ROTS			$L_2$	49.40 49.85 56.02	60.31 60.68 70.40	49.65 53.74 56.00	56.78 57.45 64.78	51.18 52.16 55.36	59.24 60.48 65.61
OPWD		uniform	cosine	52.00	68.87	52.08	61.87	52.51	64.38
WMDo		uniform	cosine	48.48	58.56	48.33	54.41	41.28	51.79
SMD	top 1 5-12 1-12	norm		61.68 62.99 60.17	61.53 62.82 59.93	59.28 <u>60.95</u> 59.79	57.94 60.82 58.91	58.42 59.07 57.47	58.32 59.32 58.24
WMD	top 1 5-12 1-12	uniform	- L <sub>2</sub>	$\begin{array}{r} 56.02\\ \underline{66.44} (\uparrow 10.42)\\ \overline{63.43} (\uparrow 7.41)\\ 62.26 (\uparrow 6.24)\end{array}$	70.40 71.36 (↑ 0.96) 70.51 (↑ 0.11) 69.88 (↓ -0.52)	56.00 58.23 († 2.23) 57.12 († 1.12) 57.78 († 1.78)	$\begin{array}{r} 64.78 \\ \underline{65.51} (\uparrow 0.73) \\ \overline{64.80} (\uparrow 0.02) \\ 64.84 (\uparrow 0.06) \end{array}$	55.36 <u>59.58</u> († 4.22) 59.43 († 4.07) 59.09 († 3.73)	65.61 65.91 ( <b>†</b> 0.30) 65.81 ( <b>†</b> 0.20) 65.62 ( <b>†</b> 0.01)
	top 1 5-12 1-12	IDF	2	55.44 65.63 († 10.19) 62.36 († 6.92) 61.24 († 5.80)	70.62 <u>71.72</u> (↑ 1.10) 70.72 (↑ 0.10) 70.03 (↓ -0.59)	55.42 57.45 (↑ 2.03) 56.37 (↑ 0.95) 56.98 (↑ 1.56)	64.48 65.26 ( <b>↑ 0.78</b> ) 64.37 (↓ -0.11) 64.40 (↓ -0.08)	50.96 53.80 (↑ 2.84) 53.40 (↑ 2.44) 52.94 (↑ 1.98)	60.24 60.33 ( <b>↑</b> 0.09) 59.93 (↓ -0.31) 59.51 (↓ -0.73)
WRD	top 1 5-12 1-12	norm	- cosine	52.01 55.04 († 3.03) 54.03 († 2.02) 54.35 († 2.34)	69.06 69.75 (↑ 0.69) 69.26 (↑ 0.20) 69.22 (↑ 0.16)	52.01 53.45 (↑ 1.44) 52.90 (↑ 0.89) 53.50 (↑ 1.49)	62.00 62.62 († 0.62) 62.17 († 0.17) 62.37 († 0.37)	52.44 54.04 (↑ 1.60) 54.12 (↑ 1.68) 54.14 (↑ 1.70)	64.75 65.05 (↑ 0.30) 65.04 (↑ 0.29) 65.01 (↑ 0.26)
	top 1 5-12 1-12	IDF		51.60 54.47 (↑ 2.87) 53.59 (↑ 1.99) 53.90 (↑ 2.30)	68.72 69.43 (↑ 0.71) 68.92 (↑ 0.20) 68.86 (↑ 0.14)	51.79 53.37 (↑ 1.58) 52.83 (↑ 1.04) 53.49 (↑ 1.70)	61.08 61.71 (↑ 0.63) 61.21 (↑ 0.13) 61.39 (↑ 0.31)	49.34 50.35 (↑ 1.01) 50.34 (↑ 1.00) 50.32 (↑ 0.98)	58.30 58.59 (↑ 0.29) 58.44 (↑ 0.14) 58.31 (↑ 0.01)
SynWMD	top 1 5-12 1-12	SWF	cosine	48.55 51.19 (↑ 2.64) 50.24 (↑ 1.69) 50.45 (↑ 1.90) 49.94	59.01 59.32 (↑ 0.31) 58.75 (↓ -0.26) 58.35 (↓ -0.66) 59.08	48.80 50.47 (↑ 1.67) 49.75 (↑ 0.95) 50.20 (↑ 1.40) 51.36	55.19 55.73 (↑ 0.54) 55.02 (↓ -0.17) 54.97 (↓ -0.22) 56.54	51.63 54.40 († 2.77) 54.47 († 2.84) 54.48 († 2.85) 54.40	64.98 65.80 († 0.82) 65.74 († 0.76) 65.49 († 0.51) 67.23
	top 1 5-12 1-12		SWD	49.94 52.11 (↑ 2.17) 51.22 (↑ 1.28) 51.31 (↑ 1.37)	59.24 ( <b>† 0.16</b> ) 58.73 ( <b>↓</b> -0.35) 58.31 ( <b>↓</b> -0.77)	52.43 († 1.07) 51.78 († 0.42) 51.95 († 0.59)	56.75 ( <b>† 0.21</b> ) 56.11 ( <b>↓</b> -0.43) 55.94 ( <b>↓</b> -0.60)	56.93 († 2.53) 56.93 († 2.53) 56.84 († 2.44)	$\frac{67.65}{67.55} (\uparrow 0.42)$ $\frac{67.55}{67.25} (\uparrow 0.32)$ $\frac{67.25}{100} (\uparrow 0.02)$

Table 20: The scores on the  $PAWS_{Wiki}$  test set for the methods using the embeddings from BERT, SimCSE, and RoBERTa. For WMD, WRD, and SynWMD, the scores of WSMD and the original method are compared for each layer selection. Score increases are highlighted in red and score decreases are highlighted in blue. Maximum scores for each embedding are underlined.

methods	layer	weight	cost	BERT0	BERT12	STSB (Spearm SimCSE0	$an's \rho \times 100)$ SimCSE12	RoBERTa0	RoBERTa12
Avg. Pool. BERTScore		uniform	-	69.16 63.27	69.07 65.13	60.83 62.90	77.54 70.59	70.25 63.38	64.09 58.71
DynaMax		IDF		63.99 71.02	65.96 71.44	63.72 68.36	70.96 77.67	64.09 70.27	59.82 66.16
SIF uSIF				68.28 68.02	69.12 68.98	57.66 57.80	76.61 76.55	68.70 69.35	64.82 64.93
Con. Neg. ROTS				68.35 68.69	69.09 69.27	60.65 61.86	77.19 77.26	69.68 69.58	64.56 64.94
OPWD		uniform	$\frac{L_2}{\text{cosine}}$	60.78 68.19	49.62 69.78	60.73 63.76	64.88 77.00	58.79 67.25	44.43
WMDo		uniform	cosine	67.61	68.74	62.17	76.18	64.63	61.16
SMD	top 1 5-12 1-12	norm		23.71 34.21 35.18	22.43 32.22 33.23	18.28 38.64 37.00	17.72 37.11 35.57	27.00 32.29 32.54	24.15 30.11 29.69
WMD	top 1 5-12 1-12	uniform	- L <sub>2</sub>	60.78 58.50 (↓ -2.28) 58.96 (↓ -1.82) 58.23 (↓ -2.55)	49.62 46.25 (↓ -3.37) 47.16 (↓ -2.46) 46.97 (↓ -2.65)	60.73 59.23 (\phi -1.50) 59.56 (\phi -1.17) 58.99 (\phi -1.74)	64.88 63.17 (↓ -1.71) 62.81 (↓ -2.07) 62.25 (↓ -2.63)	58.79 57.23 (↓ -1.56) 56.89 (↓ -1.90) 56.52 (↓ -2.27)	44.43 42.48 (↓ -1.95) 42.25 (↓ -2.18) 42.07 (↓ -2.36)
	top 1 5-12 1-12	IDF	2	64.35 62.72 (↓ -1.63) 63.10 (↓ -1.25) 62.56 (↓ -1.79)	52.98 49.86 (↓ -3.12) 50.77 (↓ -2.21) 50.85 (↓ -2.13)	64.30 63.26 (↓ -1.04) 63.71 (↓ -0.59) 63.27 (↓ -1.03)	66.27 64.74 (↓ -1.53) 64.68 (↓ -1.59) 64.40 (↓ -1.87)	62.78 61.49 (↓ -1.29) 61.27 (↓ -1.51) 61.09 (↓ -1.69)	46.97 45.04 (↓ -1.93) 45.00 (↓ -1.97) 45.05 (↓ -1.92)
WRD	top 1 5-12 1-12	norm	- cosine	70.68 70.60 (↓ -0.08) 70.65 (↓ -0.03) 70.57 (↓ -0.11)	70.30 70.02 (↓ -0.28) 70.15 (↓ -0.15) 70.15 (↓ -0.15)	65.96 65.58 (↓ -0.38) 65.65 (↓ -0.31) 65.40 (↓ -0.56)	76.87 76.83 (↓ -0.04) 76.83 (↓ -0.04) 76.82 (↓ -0.05)	69.82 69.75 (↓ -0.07) 69.71 (↓ -0.11) 69.71 (↓ -0.11)	64.09 63.63 (↓ -0.46) 63.58 (↓ -0.51) 63.56 (↓ -0.53)
	top 1 5-12 1-12	IDF		70.55 70.39 (↓ -0.16) 70.46 (↓ -0.09) 70.33 (↓ -0.22)	71.06 70.92 (↓ -0.14) 71.00 (↓ -0.06) 71.08 (↑ 0.02)	67.01 66.69 (↓ -0.32) 66.76 (↓ -0.25) 66.58 (↓ -0.43)	77.07 77.06 (↓ -0.01) 77.11 (↑ 0.04) 77.15 (↑ 0.08)	69.81 69.64 (↓ -0.17) 69.60 (↓ -0.21) 69.58 (↓ -0.23)	65.91 65.50 (↓ -0.41) 65.47 (↓ -0.44) 65.49 (↓ -0.42)
SynWMD	top 1 5-12 1-12	SWF	cosine	72.06 71.74 ( $\downarrow$ -0.32) 71.94 ( $\downarrow$ -0.12) 71.26 ( $\downarrow$ -0.80) 72.12	72.60 69.84 (↓ -2.76) 70.89 (↓ -1.71) 70.73 (↓ -1.87) 73.25	68.00 67.61 (↓ -0.39) 68.05 (↑ 0.05) 67.42 (↓ -0.58) 67.01	78.71 77.38 (↓ -1.33) 77.30 (↓ -1.41) 77.05 (↓ -1.66) 79.15	71.69 70.88 (↓ -0.81) 70.74 (↓ -0.95) 70.30 (↓ -1.39) 72.68	68.95 67.06 (↓ -1.89) 67.19 (↓ -1.76) 67.07 (↓ -1.88) 70.34
	top 1 5-12 1-12	0 1 12	SWD	$72.12 (\uparrow 0.01)  72.27 (\uparrow 0.15)  71.73 (\downarrow -0.39)$	$71.05 (\downarrow -2.20) 71.93 (\downarrow -1.32) 71.97 (\downarrow -1.28)$	66.93 (↓ -0.08) 67.45 (↑ 0.44) 66.96 (↓ -0.05)	$78.19 (\downarrow -0.96) 78.15 (\downarrow -1.00) 78.05 (\downarrow -1.10)$	$72.14 (\downarrow -0.54) 72.11 (\downarrow -0.57) 71.79 (\downarrow -0.89)$	$ \frac{70.04}{68.74} (\downarrow -1.60) \\ 68.94 (\downarrow -1.40) \\ 68.98 (\downarrow -1.36) $

Table 21: The scores on the STSB test set for the methods using the embeddings from BERT, SimCSE, and RoBERTa. For WMD, WRD, and SynWMD, the scores of WSMD and the original method are compared for each layer selection. Score increases are highlighted in red and score decreases are highlighted in blue. Maximum scores for each embedding are underlined.

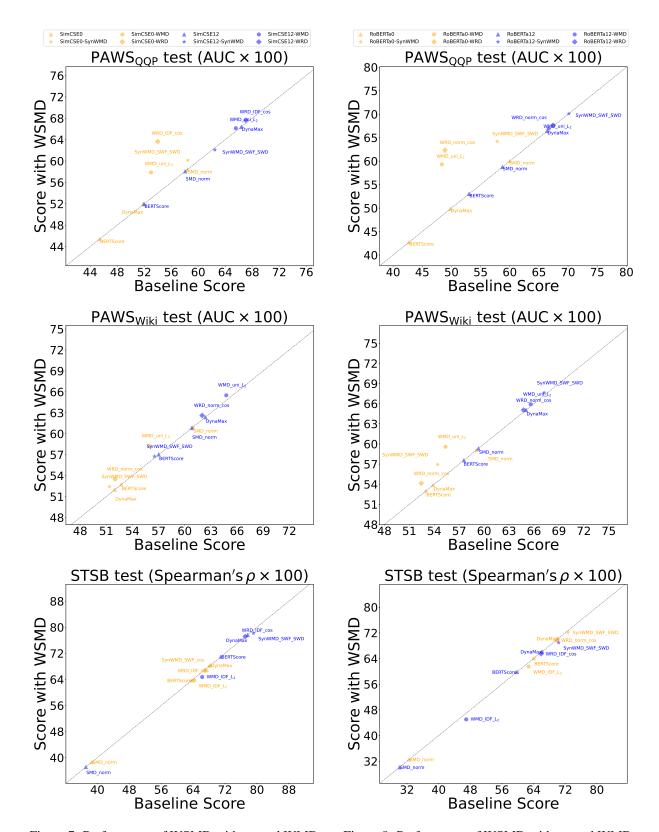


Figure 7: Performance of WSMD with several WMDlike methods (SMD, WMD, WRD, SynWMD) for Sim-CSE. The scores (AUC or Spearman's  $\rho$ ) are compared with the original WMD-like methods. Methods that are not applicable to WSMD are positioned on the diagonal line. Values above the diagonal line represent performance improvements achieved by WSMD.

Figure 8: Performance of WSMD with several WMDlike methods (SMD, WMD, WRD, SynWMD) for RoBERTa. The scores (AUC or Spearman's  $\rho$ ) are compared with the original WMD-like methods. Methods that are not applicable to WSMD are positioned on the diagonal line. Values above the diagonal line represent performance improvements achieved by WSMD.

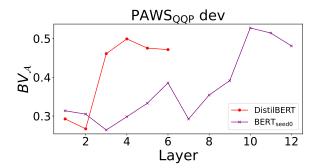


Figure 9: The layer-wise  $BV_A$  for DistilBERT and  $BERT_{seed0}$  on the PAWS<sub>QQP</sub> dev set.  $BV_A$  is high from the third layer in DistilBERT and from the fifth layer in BERT<sub>seed0</sub>.

	DistilBERT	$\text{BERT}_{\text{seed0}}$
0th Embs.	4	9
6th Embs.	4	—
12th Embs.	_	9

Table 22: Top1 layer for DistilBERT and BERT<sub>seed0</sub>. The layer was selected from the third onward for Distil-BERT and the fifth onward for BERT<sub>seed0</sub> based on the AUC of the average WSMD for a single layer using the PAWS<sub>QQP</sub> dev set.

## **G** Experiments with other models

To evaluate the generality of our method, we conducted experiments not only with BERT, SimCSE, and RoBERTa, but also with DistilBERT (Sanh et al., 2019) and BERT trained with a different seed (Sellam et al., 2022). DistilBERT is a sixlayer model distilled from BERT using BERT's weights as initialization. Since BERT has 12 layers, this initialization selects one layer from each corresponding pair of layers. For the model trained with a different seed, we chose BERT with seed 0, referred to as BERT<sub>seed0</sub>.

We used DistilBERT and  $BERT_{seed0}$  from the Hugging Face transformers library (Wolf et al., 2020) and see Table 8 in Appendix C for details.

Similar to Fig. 5, Fig. 9 shows the plots of  $BV_A$  for each layer of DistilBERT and  $BERT_{seed0}$  on the PAWS<sub>QQP</sub> dev set. For DistilBERT,  $BV_A$  is high from the third layer, while for  $BERT_{seed0}$  it is high from the fifth layer, although unlike BERT, the value decreases at the seventh layer.

Therefore, for DistilBERT, we compare performance using WMD on the  $PAWS_{QQP}$  dev set with three layer selection methods: the best single layer

from the third (top1 layer), third to sixth (3-6 layers), and all layers (1-6 layers). For  $BERT_{seed0}$ , we compare performance using the same three settings as for BERT on the  $PAWS_{QQP}$  dev set.

Table 22 shows the top1 layer for each model.

The scores for methods that depend on word embeddings are shown in Tables 23, 24, and 25.

## H Experiments with SICK-R

In addition to STSB, we also extended our experiments to another dataset, SICK-R (Marelli et al., 2014), using BERT to measure semantic textual similarity.

Similar to STSB, SICK-R contains humanannotated scores for English sentence pairs, reflecting the average similarity on a six-point scale.

Table 26 shows the number of sentence pairs in the SICK-R test set.

The scores for methods that depend on word embeddings are shown in Table 27.

### I Experiments with PAWS<sub>QQP</sub> train set

As seen in Section 7.7, the size of the  $PAWS_{QQP}$  test set is small and the dataset contains only 677 sentence pairs. To alleviate this problem, we present the scores on the  $PAWS_{QQP}$  train set using our method.

Table 28 shows the number of sentence pairs in the  $PAWS_{QQP}$  train set.

The scores for methods that depend on word embeddings are shown in Table 29.

It should be noted that the top layer was determined based on the first 1500 sentence pairs, so it implies a potential bias in the layer selection.

# J Correlation between common words count and gold score in sentence pairs.

For PAWS<sub>QQP</sub>, PAWS<sub>Wiki</sub>, and STSB, We present scatter plots of the number of common words in sentence pairs against their respective gold scores in Fig. 10. Compared to PAWS, STSB shows a strong correlation between the number of common words and the gold score. Therefore, in STSB, there is no need to worry about a gold score decrease for sentence pairs with high word overlap. This suggests that even when sentences are considered as sets of words, good performance can be achieved.

methods	layer	weight	cost	DistilBERT0	PAWS <sub>QQP</sub> (. DistilBERT12	$AUC \times 100)$ BERT <sub>seed0</sub> 0	$BERT_{seed0}12$
Avg. Pool. BERTScore DynaMax SIF uSIF Con. Neg. ROTS OPWD		uniform IDF uniform		52.02 45.58 45.46 52.02 52.26 52.29 52.15 51.71 53.03	63.22 54.74 55.30 70.00 63.03 63.06 63.12 64.95 67.33	52.80 45.50 45.41 54.59 52.79 52.85 52.64 55.25 53.53	63.94 52.05 52.46 66.71 63.68 63.60 63.76 64.37 66.99
WMDo		uniform	cosine cosine	54.73 44.18	$\frac{70.93}{55.42}$	55.69 44.07	68.43 58.53
WMD	top 1 5-12 1-12	uniform	- L <sub>2</sub>	53.03 59.47 (↑ 6.44) 58.87 (↑ 5.84) 59.01 (↑ 5.98) 52.44	67.33 66.99 (↓ -0.34) 67.52 (↑ 0.19) 67.38 (↑ 0.05) 66.79	$53.53$ $71.95 (\uparrow 18.42)$ $66.64 (\uparrow 13.11)$ $65.25 (\uparrow 11.72)$ $53.06$	66.99 67.24 (↑ 0.25) 67.45 (↑ 0.46) 67.59 (↑ 0.60) 66.69
	top 1 5-12 1-12	IDF		58.41 († 5.97) 57.97 († 5.53) 58.07 († 5.63)	66.33 (↓ -0.46) 66.98 (↑ 0.19) 66.87 (↑ 0.08)	70.80 († 17.74) 65.63 († 12.57) 64.18 († 11.12)	67.35 ( <b>↑</b> 0.66) 67.23 ( <b>↑</b> 0.54) 67.29 ( <b>↑</b> 0.60)
WRD	top 1 5-12 1-12	norm	cosine	53.25 63.02 (↑ 9.77) 62.88 (↑ 9.63) 62.95 (↑ 9.70)	70.39 70.35 (↓ -0.04) 70.51 (↑ 0.12) 70.50 (↑ 0.11)	56.00 71.65 († 15.65) 68.56 († 12.56) 68.27 († 12.27)	67.56 67.93 († 0.37) 67.79 († 0.23) 68.00 († 0.44)
	top 1 5-12 1-12	IDF		54.46 64.37 (↑ 9.91) <u>65.08</u> (↑ 10.62) 64.97 (↑ 10.51)	70.59 70.46 (↓ -0.13) 70.74 (↑ 0.15) 70.71 (↑ 0.12)	55.49 71.83 († 16.34) 68.85 († 13.36) 68.71 († 13.22)	68.32 68.63 (↑ 0.31) 68.49 (↑ 0.17) <u>68.67</u> (↑ 0.35)
SynWMD	top 1 5-12 1-12	SWF	cosine	47.43 54.58 (↑ 7.15) 56.21 (↑ 8.78) 55.76 (↑ 8.33) 58.43	$60.9859.40 (\downarrow -1.58)60.47 (\downarrow -0.51)60.17 (\downarrow -0.81)64.47$	47.47 64.53 († 17.06) 60.43 († 12.96) 59.66 († 12.19) 59.51	60.52 60.29 (↓ -0.23) 60.17 (↓ -0.35) 60.27 (↓ -0.25) 65.29
	top 1 5-12 1-12		SWD	59.73 († 1.30) 60.09 († 1.66) 60.06 († 1.63)	$64.47 \\ 62.80 (\downarrow -1.67) \\ 63.73 (\downarrow -0.74) \\ 63.50 (\downarrow -0.97)$	66.72 († 7.21) 63.84 († 4.33) 63.08 († 3.57)	$\begin{array}{c} 63.29\\ 63.38 (\downarrow -1.91)\\ 63.94 (\downarrow -1.35)\\ 64.18 (\downarrow -1.11) \end{array}$

Table 23: The scores on the  $PAWS_{QQP}$  test set for the methods using the embeddings from DistilBERT and  $BERT_{seed0}$ . For WMD, WRD, and SynWMD, the scores of WSMD and the original method are compared for each layer selection. Score increases are highlighted in red and score decreases are highlighted in blue. Maximum scores for each embedding are underlined.

methods	layer	weight	cost	DistilBERT0	PAWS <sub>Wiki</sub> ( DistilBERT12	${ m AUC}  imes 100) \\ { m BERT}_{ m seed0} 0$	BERT <sub>seed0</sub> 12
Avg. Pool. BERTScore DynaMax SIF uSIF Con. Neg. ROTS OPWD		uniform IDF uniform	$\frac{L_2}{\text{cosine}}$	50.17 52.58 52.73 50.10 50.05 50.11 54.93 55.78 51.98	57.25 56.08 56.12 59.34 57.09 57.20 57.44 57.68 69.95 66.96	49.93 52.60 52.68 52.50 49.89 49.86 49.89 54.76 55.69 52.33	$\begin{array}{c} 60.22\\ 57.21\\ 57.32\\ 56.44\\ 60.00\\ 60.16\\ 60.55\\ 60.62\\ 70.90\\ 68.76\end{array}$
WMDo		uniform	cosine	48.45	57.16	48.62	58.79
WMD	top 1 5-12 1-12	uniform	- L <sub>2</sub>	55.78 <u>58.64</u> (↑ 2.86) <u>58.15</u> (↑ 2.37) <u>58.63</u> (↑ 2.85)	69.95 64.85 (↓ -5.10) 69.20 (↓ -0.75) 68.79 (↓ -1.16)	55.69 <u>68.26</u> († 12.57) 64.10 († 8.41) 62.11 († 6.42)	70.90 68.56 ( $\downarrow$ -2.34) 69.16 ( $\downarrow$ -1.74) 68.30 ( $\downarrow$ -2.60)
	top 1 5-12 1-12	IDF	-2	55.20 57.58 († 2.38) 57.36 († 2.16) 57.80 († 2.60)	$\frac{70.19}{64.36 (\downarrow -5.83)} \\ 69.36 (\downarrow -0.83) \\ 68.93 (\downarrow -1.26)$	55.18 67.10 (↑ 11.92) 63.00 (↑ 7.82) 61.06 (↑ 5.88)	$\frac{71.15}{69.42 (\downarrow -1.73)} \\ 69.80 (\downarrow -1.35) \\ 68.63 (\downarrow -2.52)$
WRD	top 1 5-12 1-12	norm	- cosine	52.21 54.75 (↑ 2.54) 53.98 (↑ 1.77) 54.34 (↑ 2.13)	67.07 66.83 (↓ -0.24) 67.28 (↑ 0.21) 67.32 (↑ 0.25)	52.45 60.15 († 7.70) 57.44 († 4.99) 56.62 († 4.17)	68.79 69.50 (↑ 0.71) 69.16 (↑ 0.37) 68.99 (↑ 0.20)
	top 1 5-12 1-12	IDF		51.76 54.39 (↑ 2.63) 53.73 (↑ 1.97) 54.11 (↑ 2.35)	66.69 66.28 (↓ -0.41) 66.89 (↑ 0.20) 66.92 (↑ 0.23)	52.08 59.70 (↑ 7.62) 57.15 (↑ 5.07) 56.38 (↑ 4.30)	68.72 69.55 († 0.83) 69.15 († 0.43) 68.93 († 0.21)
SynWMD	top 1 5-12 1-12	SWF	cosine	48.90 51.00 (↑ 2.10) 50.81 (↑ 1.91) 51.09 (↑ 2.19)	57.08 55.20 ( $\downarrow$ -1.88) 56.83 ( $\downarrow$ -0.25) 56.70 ( $\downarrow$ -0.38)	48.69 56.64 (↑ 7.95) 53.93 (↑ 5.24) 52.85 (↑ 4.16)	$59.52$ $59.07 (\downarrow -0.45)$ $58.82 (\downarrow -0.70)$ $58.47 (\downarrow -1.05)$
	top 1 5-12 1-12		SWD	52.28 52.45 (↑ 0.17) 53.14 (↑ 0.86) 53.20 (↑ 0.92)	57.10 55.09 (\-2.01) 56.73 (\-0.37) 56.58 (\-0.52)	52.06 57.08 (↑ 5.02) 55.11 (↑ 3.05) 54.18 (↑ 2.12)	59.11 58.64 (↓ -0.47) 58.40 (↓ -0.71) 58.06 (↓ -1.05)

Table 24: The scores on the  $PAWS_{Wiki}$  test set for the methods using the embeddings from DistilBERT and  $BERT_{seed0}$ . For WMD, WRD, and SynWMD, the scores of WSMD and the original method are compared for each layer selection. Score increases are highlighted in red and score decreases are highlighted in blue. Maximum scores for each embedding are underlined.

methods	layer	weight	cost			$an's \rho \times 100)$	
methods	layer	weight	cost	DistilBERT0	DistilBERT12	$BERT_{seed0}0$	BERT <sub>seed0</sub> 12
Avg. Pool.				66.33	71.83	61.98	51.78
BERTScore		uniform		63.30	63.01	63.31	60.15
DynaMax		IDF		64.16 70.61	63.92 72.66	64.22 69.35	$\frac{60.97}{51.05}$
SIF				65.35	72.00	<u>59.20</u>	47.38
uSIF				65.25	71.64	59.34	47.40
Con. Neg.				65.81	71.86	61.76	52.44
ROTS				66.61	71.98	62.94	52.90
OPWD		uniform	$L_2$	60.59	52.63	61.05	42.70
OPWD		uniform	cosine	67.29	70.93	64.74	48.08
WMDo		uniform	cosine	66.59	70.13	63.48	42.52
				60.59	52.63	61.05	42.70
	top 1	uniform		52.78 ( <b>J</b> -7.81)	44.94 ( <b>↓ -7.69</b> )	51.13 ( <b>J</b> -9.92)	34.24 ( <b>J</b> -8.46)
	5-12	unitorin		58.50 ( <b>↓</b> - <b>2.09</b> )	50.04 ( <b>J</b> -2.59)	56.31 (↓ -4.74)	40.36 (↓ -2.34)
WMD	1-12		- L <sub>2</sub>	58.07 ( <b>↓</b> -2.52)	49.52 ( <b>↓</b> - <b>3</b> .11)	56.69 ( <b>J</b> - <b>4.36</b> )	41.25 (↓ -1.45)
			112	64.36	55.98	64.64	45.31
	top 1	IDF		58.30 (↓ -6.06)	49.73 (↓ -6.25)	56.22 (↓ -8.42)	37.72 (↓ -7.59)
	5-12 1-12			$62.85 (\downarrow -1.51)$ $62.53 (\downarrow -1.83)$	$53.83 (\downarrow -2.15)$ $53.38 (\downarrow -2.60)$	$61.26 (\downarrow -3.38)$ $61.60 (\downarrow -3.04)$	$44.62 (\downarrow -0.69)$ $45.42 (\uparrow 0.11)$
	1-12			02.33 (4 -1.83)	33.38 (4 -2.00)	01.00 (↓ -3.04)	43.42 (  0.11)
				69.73	71.30	67.06	47.85
	top 1	norm		68.57 (↓ -1.16)	70.23 (↓ -1.07)	64.09 ( <b>↓</b> - <b>2.97</b> )	44.35 (↓ -3.50)
	5-12	norm		69.54 ( <b>↓</b> -0.19)	71.13 ( <b>↓</b> -0.17)	65.67 (↓ -1.39)	46.14 (↓ -1.71)
WRD	1-12		cosine	69.47 ( <b>↓</b> -0.26)	71.09 ( <b>↓</b> -0.21)	65.72 ( <b>↓</b> -1.34)	46.26 (↓ -1.59)
	ton 1			69.89 68.65 (↓ -1.24)	72.23 71.45 ( <b>J</b> - <b>0.78</b> )	67.85 65.16 (↓ -2.69)	50.67 47.34 (↓ -3.33)
	top 1 5-12	IDF		$69.65 (\downarrow -0.24)$	$71.43 (\downarrow -0.78)$ $72.16 (\downarrow -0.07)$	$66.62 (\downarrow -1.23)$	$47.34 (\downarrow -3.33)$ $49.08 (\downarrow -1.59)$
	1-12			$69.56 (\downarrow -0.33)$	$72.10 (\downarrow -0.07)$ $72.14 (\downarrow -0.09)$	66.69 (↓ -1.16)	$49.08 (\downarrow -1.39)$ $49.18 (\downarrow -1.49)$
				71.56	73.90	69.30	54.21
	top 1 5-12		cosine	67.79 (↓ -3.77) 71.00 (↓ -0.56)	$68.76 (\downarrow -5.14)$ 72.36 ( $\downarrow -1.54$ )	64.20 (↓ -5.10) 67.03 (↓ -2.27)	44.35 (↓ -9.86) 49.75 (↓ -4.46)
	1-12			$71.00 (\downarrow -0.30)$ $70.69 (\downarrow -0.87)$	$72.05 (\downarrow -1.85)$	$67.03 (\downarrow -2.27)$ $67.10 (\downarrow -2.20)$	$50.02 (\downarrow -4.19)$
SynWMD	1-12	SWF		70.89 (1 -0.87)	74.67	68.52	57.09
	top 1			68.30 ( <b>↓</b> -2.56)	$71.23 (\downarrow -3.44)$	65.54 (↓ -2.98)	49.22 (1 -7.87)
	5-12		SWD	$70.76 (\downarrow -0.10)$	73.52 (1 -1.15)	67.32 (1 -1.20)	54.02 (1 -3.07)
	1-12			70.55 (↓ -0.31)	73.31 (↓ -1.36)	67.34 (↓ -1.18)	54.34 (↓ -2.75)
	5-12		SWD	70.76 ( <b>↓</b> -0.10)	73.52 (↓ -1.15)	67.32 (↓ -1.20)	54.02 (↓ -3.07

Table 25: The scores on the STSB test set for the methods using the embeddings from DistilBERT and BERT<sub>seed0</sub>. For WMD, WRD, and SynWMD, the scores of WSMD and the original method are compared for each layer selection. Score increases are highlighted in red and score decreases are highlighted in blue. Maximum scores for each embedding are underlined.

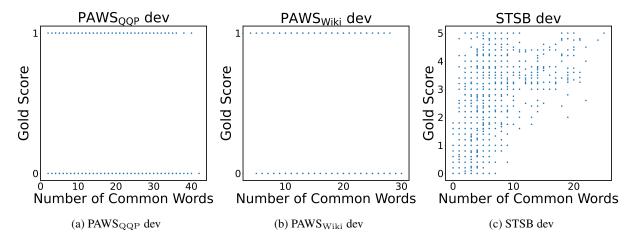


Figure 10: Scatter plots of the number of common words in sentence pairs for each dataset against the corresponding gold scores. (a) Spearman's  $\rho \times 100 = -9.31$  for the PAWS<sub>QQP</sub> dev set. (b) Spearman's  $\rho \times 100 = -0.85$  for the PAWS<sub>Wiki</sub> dev set. (c) Spearman's  $\rho \times 100 = 59.37$  for STSB dev set.

	Test		
SICK-R	4927		

Table 26: The number of sentence pairs in the SICK-R test set.

	1	weight		SICK-R (Spearman's $\rho \times 100$ )		
methods	layer		cost	BERT0	BERT12	
Avg. Pool.				44.10	62.19	
BERTScore		uniform		50.29	58.55	
		IDF		50.54	58.26	
DynaMax				48.38	61.99	
SIF				43.02	61.95	
uSIF				42.93	61.92	
Con. Neg.				44.34	62.30	
ROTS			_	44.46	62.26	
OPWD		uniform	L_2	49.97	54.06	
			cosine	48.49	61.72	
WMDo		uniform	cosine	36.93	60.70	
		uniform		49.97	54.06	
	top 1			50.13 ( <b>† 0.16</b> )	53.39 ( <b>↓</b> -0.67)	
	5-12	unnorm		50.14 ( <b>†</b> 0.17)	53.41 ( <b>↓</b> -0.65)	
WMD	1-12		$L_2$	50.07 ( <b>†</b> 0.10)	53.04 ( <b>1.02</b> )	
WIND			112	49.39	53.55	
	top 1	IDF		49.58 ( <b>† 0.19</b> )	52.99 ( <b>↓</b> -0.56)	
	5-12	101		49.53 ( <b>† 0.14</b> )	52.94 ( <b>↓</b> -0.61)	
	1-12			49.48 ( <b>† 0.09</b> )	52.57 ( <b>↓</b> - <b>0.98</b> )	
				47.78	61.62	
	top 1	norm		47.77 ( <b>↓</b> - <mark>0.01</mark> )	61.51 ( <b>↓</b> -0.11)	
	5-12	norm		47.75 ( <b>↓</b> - <b>0.03</b> )	61.48 ( <b>↓</b> -0.14)	
WRD	1-12		cosine	47.69 ( <b>↓</b> - <mark>0.09</mark> )	61.34 ( <b>↓</b> -0.28)	
WKD			cosine	48.13	61.29	
	top 1	IDF		48.08 ( <b>↓</b> - <b>0.05</b> )	61.20 ( <b>↓</b> -0.09)	
	5-12	ibi		48.05 ( <b>↓</b> - <b>0.08</b> )	61.15 ( <b>↓</b> -0.14)	
	1-12			47.98 ( <b>↓</b> -0.15)	61.02 ( <b>↓</b> -0.27)	
				50.52	63.35	
	top 1		cosine	<u>50.65</u> ( <b>† 0.13</b> )	62.49 ( <b>↓</b> -0.86)	
	5-12	SWF		50.47 (↓ -0.05)	62.35 ( -1.00)	
SUNWMD	1-12			50.38 (↓ -0.14)	61.97 (↓ -1.38)	
SynWMD		SWF		49.59	63.54	
	top 1		SWD	49.92 ( <b>† 0.33</b> )	62.96 ( <b>↓</b> -0.58)	
	5-12			49.70 ( <b>† 0.11</b> )	62.78 ( <b>↓</b> -0.76)	
	1-12			49.70 ( <b>† 0.11</b> )	62.52 ( <b>↓</b> -1.02)	

Table 27: The scores on the SICK-R test set for the methods using the BERT embeddings. For WMD, WRD, and SynWMD, the scores of WSMD and the original method are compared for each layer selection. Score increases are highlighted in red and score decreases are highlighted in blue. Maximum scores for each embedding are underlined.

	Train		
$\text{PAWS}_{\mathrm{QQP}}$	11988 (31.50%)		

Table 28: The number of sentence pairs in the  $PAWS_{\rm QQP}$  train set. The percentage of paraphrases is shown in parentheses.

methods	layer wei	weight	cost	$PAWS_{QQP}$ train (AUC × 100)					
		neight	0051	BERT0	BERT12	SimČSE0	SimCSE12	RoBERTa0	RoBERTa12
Avg. Pool.				66.14	75.57	66.84	73.92	61.58	73.73
BERTScore		uniform		50.41	58.79	50.61	52.59	45.65	57.97
		IDF	-	50.74	58.51	50.73	52.52	48.21	59.33
DynaMax				67.61	79.25	68.12	73.42	63.56	71.49
SIF				65.80	75.28	66.24	73.34	61.58	73.04
uSIF				65.89	75.28	66.22	73.36	61.67	72.99
Con. Neg.				66.03	75.64	66.48	74.04	61.60	73.69
ROTS				60.46	76.59	61.13	74.55	54.91	74.01
OPWD		uniform	$L_2$	67.65	77.90	67.77	75.49	64.35	76.98
OF WD		unitorni	cosine	68.92	79.73	68.80	75.91	66.21	76.46
WMDo		uniform	cosine	49.84	61.95	49.85	53.28	59.53	68.86
				67.65	77.90	67.77	75.49	64.35	76.98
	top 1*	·····		79.42 († 11.77)	78.43 ( <b>† 0.53</b> )	74.81 (↑ 7.04)	76.04 ( <b>†</b> 0.55)	73.61 ( <u>† 9.26</u> )	77.02 ( <b>↑ 0.04</b> )
	5-12	uniform	uniform	76.49 (	78.13 ( <b>† 0.23</b> )	75.11 († 7.34)	75.75 ( <b>† 0.26</b> )	<u>73.70</u> ( <b>† 9.35</b> )	76.98 (-)
WMD	1-12			76.49 ( <u>* 8.84</u> )	78.10 ( <b>† 0.20</b> )	76.13 ( <b>† 8.36</b> )	76.04 ( <b>† 0.55</b> )	73.06 (  8.71)	76.65 ( <b>↓</b> -0.33)
W WID			L <sub>2</sub>	67.41	77.54	67.53	75.28	64.67	76.12
	top 1*	IDF		78.88 (↑ 11.47)	78.16 ( <u>10.62</u> )	75.22 ( <b>† 7.69</b> )	75.86 ( <u>† 0.58</u> )	73.03 ( <u>† 8.36</u> )	76.26 ( <b>↑</b> 0.14)
	5-12	IDF	IDF	75.88 ( <b>† 8.47</b> )	77.80 ( <b>†</b> 0.26)	74.66 († 7.13)	75.53 ( <b>†</b> 0.25)	73.05 (↑ 8.38)	76.08 ( <b>↓</b> -0.04)
	1-12			75.99 ( <b>† 8.58</b> )	77.79 ( <mark>† 0.25</mark> )	75.85 ( <b>† 8.32</b> )	75.84 ( <mark>† 0.56</mark> )	72.43 ( <b>† 7.76</b> )	75.70 ( <b>↓</b> -0.42)

Table 29: The scores on the  $PAWS_{QQP}$  train set for the methods using the embeddings from BERT, SimCSE, and RoBERTa. For WMD, the scores of WSMD and the original method are compared for each layer selection. Score increases are highlighted in red and score decreases are highlighted in blue. Maximum scores for each embedding are underlined. Note that the top layer was determined based on the first 1500 sentence pairs. For this reason, *top1* is marked with an asterisk.