Bidirectional Attention as a Mixture of Continuous Word Experts

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Abstract

Bidirectional attention-composed of self-attention with positional encodings and the masked language model (MLM) objective-has emerged as a key component of modern large language models (LLMs). Despite its empirical success, few studies have examined its statistical underpinnings: What statistical model is bidirectional attention implicitly fitting? What sets it apart from its non-attention predecessors? We explore these questions in this paper. The key observation is that fitting a single-layer single-head bidirectional attention, upon reparameterization, is equivalent to fitting a continuous bag of words (CBOW) model with mixture-of-experts (MOE) weights. Further, bidirectional attention with multiple heads and multiple layers is equivalent to stacked MOEs and a mixture of MOEs, respectively. This statistical viewpoint reveals the distinct use of MOE in bidirectional attention, which aligns with its practical effectiveness in handling heterogeneous data. It also suggests an immediate extension to categorical tabular data, if we view each word location in a sentence as a tabular feature. Across empirical studies, we find that this extension outperforms existing tabular extensions of transformers in out-of-distribution (OOD) generalization. Finally, this statistical perspective of bidirectional attention enables us to theoretically characterize when linear word analogies are present in its word embeddings. These analyses show that bidirectional attention can require much stronger assumptions to exhibit linear word analogies than its non-attention predecessors.¹

Keywords: bidirectional attention, large language models, mixture of experts.

¹Software that replicates the empirical studies can be found at https://github.com/yixinw-lab/ attention-uai.

1 Introduction

First introduced by Vaswani et al. [2017], bidirectional attention represents a departure from the traditional recurrent or convolutional neural networks in language modeling. This architecture has since become the backbone of many large language models, including BERT [Devlin et al., 2019], RoBERTa [Liu et al., 2019], and GPT-2 [Radford et al., 2019], all of which have achieved exceptional performance in natural language processing benchmarks.

At the heart of bidirectional attention lies the self-attention mechanism: it creates a holistic representation of each sentence by capturing pairwise relationships between tokens in the sentence. Equally important are positional encodings, supplying word ordering information that allows bidirectional attention to move beyond bag-of-words. Finally, bidirectional attention employs the masked language model (MLM) objective, a self-supervised learning objective for unlabelled text data which minimizes the model's cross-entropy loss for predicting randomly masked words within each sentence.

Despite the empirical success of attention-based language models, few works have examined their statistical underpinnings: What statistical models are these attention-based models implicitly fitting? What sets these models apart from their non-attention predecessors like continuous bag of words (CBOW) [Mikolov et al., 2013]? How does the use of the self-attention mechanism contribute to these models' empirical success? We explore these questions in this work.

Main ideas and contributions. In this paper, we conduct a theoretical investigation into bidirectional attention. The key observation is that upon reparameterization, fitting a single-head and single-layer bidirectional attention is equivalent to fitting CBOW with mixture-of-experts (MOE) weights [Jacobs et al., 1991]. Moreover, bidirectional attention with multiple heads and multiple layers is equivalent to stacked MOEs and a mixture of MOEs, respectively. These analyses reveal the distinct use of MOE in bidirectional attention as compared with its non-attention predecessors. In particular, they partially explain the practical effectiveness of bidirectional attention in capturing heterogeneous natural language patterns [Devlin et al., 2019, Liu et al., 2019].

This statistical interpretation of bidirectional attention suggests an immediate extension to modeling (categorical) tabular data: one can view each word position in a sentence as a tabular feature, and each word as the value that the feature takes. Across empirical studies, we find that this tabular extension improves out-of-distribution (OOD) generalization compared with existing tabular data algorithms or tabular extensions of attention. Moreover, this extension may facilitate the integration of heterogeneous data sets with partially overlapping features: the learned feature encodings (akin to positional encodings in the original attention module) bring all features into the same embedding space.

Finally, the connection between bidirectional attention and CBOW+MOE empowers us to theoretically characterize when linear word analogies (e.g. king - man + woman \approx queen) can be present in its word embeddings. We draw on a classical finding in Levy and Goldberg [2014]: the similarity between two tokens from word2vec embeddings is equal to their pointwise mutual information [Church and Hanks, 1990], provided that the embeddings have sufficient dimensionality and the models are trained using the skip-gram with negative sampling (SGNS) objective. This result enables us to analyze the embeddings of bidirectional attention through its connection to CBOW. Adopting the paraphrasing argument of Allen and Hospedales [2019] for SGNS, we characterize the conditions under which both CBOW and attention-based embeddings exhibit linear word analogies. We show that bidirectional attention can require much stronger conditions than its non-attention predecessors. These results partially explain the empirical observations that bidirectional attention may not always achieve meaningful improvements over classical word embeddings in capturing abstract and complex relationships [Ushio et al., 2021].

Related work. Our work draws on three themes around attention-based models.

The first is a body of work on the *theoretical foundations of attention-based models*. Elhage et al. [2021] analyzed how the different components of decoder-only attention-based architectures relate to each other. Edelman et al. [2022] provided a rigorous justification of the ability of attention-based architectures to represent sparse functions. Tsai et al. [2019] viewed attention through the perspective of kernels. Peng et al. [2020] established a connection between the use of multiple heads in transformers and MOE. Li et al. [2023] showed that the embedding and self-attention layers in a transformer architecture are capable of capturing topic structures.

More recently, numerous studies have been devoted to unraveling the reasons behind the exceptional performance of attention-based models, such as transformers, at in-context learning from various viewpoints. For instance, Akyürek et al. [2022], Bai et al. [2023], Dai et al. [2023], Von Oswald et al. [2023], Zhang et al. [2023], and Ahn et al. [2023] attributed this intriguing phenomenon to transformers' capability to implement gradient descent. Alternatively, studies by Xie et al. [2021], Ahuja et al. [2023], and Wang et al. [2023] approached the explanation from a Bayesian perspective. In contrast to these works, we provide a statistical interpretation of the bidirectional attention objective, showing that fitting a single-layer single-head attention-based architecture is equivalent to fitting a CBOW model with MOE weights; this statistical interpretation provides a theoretical basis for the empirical effectiveness of bidirectional attention in handling heterogeneous data [Devlin et al., 2019, Liu et al., 2019].

The second theme is the *extension of attention-based models to tabular data*. One prominent work along this line is TabTransformer [Huang et al., 2020], which utilizes a concatenation of token embeddings and unique feature identifiers—in lieu of positional encodings—to learn contextual embeddings for categorical features with self-attention. Different from TabTransformer, we view each word location in a sentence as a tabular feature; our extension thus represents each feature in tabular data via an encoding akin to the positional encodings. Other tabular extensions of self-attention include FTTransformer (tokenizing each feature, applying transformer layers, and using the [CLS] token for prediction) [Gorishniy et al., 2021], AutoInt (mapping all features into the same space and applying self-attention to model between-feature interactions) [Song et al., 2019] and TabNet (utilizing sequential attention for feature selection in different learning steps) [Arik and Pfister, 2021]. Compared with these existing approaches, our approach is more robust to covariate shifts across empirical studies; it also facilitates the integration of heterogeneous datasets with partially overlapping features.

The third theme relates to *linear word analogy structures in word embeddings*. Neural word embeddings such as word2vec [Mikolov et al., 2013] and GloVe [Pennington et al., 2014] have been empirically shown to exhibit linear structures as manifested through analogies. Concretely, given an analogy "*a* is to *b* as *c* is to *d*", we often find $w_b + w_c - w_a \approx w_d$, where w_i denotes the embedding

of word $i \in \{a, b, c, d\}$. Many works provide theoretical justifications for this phenomenon. Arora et al. [2016] offered a latent variable argument, assuming that texts are generated from random walks of discourse vectors and word vectors are spatially isotropic. Ethayarajh et al. [2019] introduced the *co-occurrence shifted PMI* concept which characterizes when linear analogy holds in sGNs and GloVe. Allen and Hospedales [2019] adopted the paraphrasing framework of Gittens et al. [2017] and used *word transformation* to connect linear analogy in sGNs with paraphrases. In contrast to these existing works, our work moves beyond sGNs and GloVe; we characterize when linear word analogies may be present in CBOW and attention-based embeddings.

2 Bidirectional attention as a mixture of continuous word experts

In this section, we first review bidirectional attention, a model composed of the self-attention architecture, positional encodings, and the MLM training objective. En route, we derive an explicit form of the MLM objective for a single-layer single-head attention-based architecture in Section 2.1. We then formally establish the equivalence between fitting bidirectional attention and fitting the CBOW model with MOE weights in Section 2.2, with extensions to multi-head and multi-layer attention-based architectures.

2.1 Bidirectional attention: Self-attention, positional encodings, and the MLM objective

We begin with describing the structure of bidirectional attention—self-attention, positional encodings, and the MLM objective—in the context of language modeling. (Appendix A contains a summary of the notations used in this section.)

Building blocks of bidirectional attention. Consider a corpus that consists of sentences of length S, with a vocabulary size of |V|. The self-attention mechanism takes sentences and outputs their sentence embeddings, by transforming the token embeddings and positional encodings of each token in the sentence. We denote $C \in \mathbb{R}^{(|V|+1) \times p}$ as the matrix such that each row c_i^{\top} corresponds to the token embedding of the *i*-th token in the vocabulary. The (|V|+1)-th token is the [MASK] token, representing a token in the training corpus that is masked. We further denote $P \in \mathbb{R}^{S \times p}$ as the positional encoding matrix.

To learn these token embeddings and positional encodings, bidirectional direction employs an MLM objective: it randomly masks a random subset of the tokens in the training corpus; then it aims to predict these masked tokens from the sentence embeddings, which are produced by transforming the token embeddings and positional encodings through the attention mechanisms. To operationalize the MLM objective, we use $\overline{X} \in \{0,1\}^{S \times (|V|+1)}$ to denote the one-hot encoding matrix of the S tokens (including the masked tokens) in each sentence. For notational simplicity, we consider a simple masking strategy: each sentence produces S prediction tasks in the MLM objective, each of which involves masking exactly one of the S positions in the sentence and predicting the token in that position. (Results in this section can be easily generalized to general masking strategies.)

Predicting masked tokens with self-attention. We next describe how the self-attention mechanism with positional encodings produces predictions of masked tokens. For ease of exposition, we focus on a single-head single-layer attention module. It takes in \overline{X} , the one-hot encoding matrix of the S tokens in a sentence (including the masked tokens); it then outputs a probability vector $\hat{y} \in \Delta^{|V|}$ as the prediction for the masked token, indicating the probability of the masked token being each of the |V| words in the vocabulary.

The self-attention architecture transforms \overline{X} into the prediction \hat{y} through the following steps:

- 1. Token embeddings with positional encodings. We produce a matrix consisting of the token embeddings of all the tokens in the masked sentence: $X = \overline{X}C \in \mathbb{R}^{S \times p}$. We then add positional encodings to the matrix: X' = X + P.
- 2. Sentence embeddings with attention weight matrices: Employing the value mapping $W^V \in \mathbb{R}^{d \times p}$, query mapping $W^Q \in \mathbb{R}^{d_w \times p}$, and key mapping $W^K \in \mathbb{R}^{d_w \times p}$, we obtain the sentence embedding $X^{\text{attn}} \in \mathbb{R}^{S \times d}$ after applying the attention weights:

$$X^{\text{attn}} = \text{softmax}\left(\frac{X'(W^Q)^\top W^K(X')^\top}{\sqrt{d_w}}\right) X'(W^V)^\top.$$

Here, the softmax is taken row-wise.

- 3. Intermediate representations with a residual connection. We then obtain an intermediate representation with the coefficient matrix $W^O \in \mathbb{R}^{d \times p}$: $Z = X^{\text{attn}} W^O \in \mathbb{R}^{S \times p}$. This is followed by a residual connection: $Z' = X' + Z \in \mathbb{R}^{S \times p}$.
- 4. Final predictions with a linear layer and residual connection. For each position i ∈ [S] of the sentence, we apply a linear layer LIN₁(Z'_i) = W'Z'_i ∈ ℝ^p with a weight matrix W' ∈ ℝ^{p×p}. We then apply another residual connection: Z" = Z' + LIN₁(Z') ∈ ℝ^{S×p}. Finally, we employ another linear layer and the softmax operation:

$$\hat{y} = \operatorname{softmax}(\operatorname{LIN}_2(Z_i'')),$$

where $\operatorname{LIN}_2(Z_i'') = W''Z_i'' \in \mathbb{R}^{|V|}$ with a weight matrix $W'' \in \mathbb{R}^{|V| \times p}$.

Given the self-attention transformation from an input sentence \overline{X} to a probability vector \hat{y} which predicts the masked token, bidirectional attention learns the token embeddings, positional encodings, and weight matrices by optimizing the cross entropy loss of \hat{y} in predicting the masked token. This loss objective is also known as the MLM objective.

The loss objective of bidirectional attention. We next derive an explicit form for the loss objective of bidirectional attention. This derivation will pave the road for the statistical interpretation of bidirectional attention.

In more detail, we consider an input-output pair $(\overline{X}, \overline{y})$ for the masked token prediction task, where \overline{X} is the one-hot encoding matrix of all tokens in the sentence, and $\overline{y} \in \{0, 1\}^{|V|}$ is the one-hot encoding of the masked token. We denote $m \in [S]$ and $b \in [|V|]$ as the masked position and masked token, respectively. Lemma 1 below derives an explicit form of the MLM objective $L_{\text{MLM}}(m, b)$.

Lemma 1 (The loss objective of bidirectional attention). Upon reparameterization, the MLM objective for predicting token *b* in the *m*-th position is given by

$$L_{\text{MLM}}(m,b) = -\frac{\sum_{j=1}^{S} \theta(j,m) \chi(j,m,b)}{\sum_{j=1}^{S} \theta(j,m)} + \log\left(\sum_{k=1}^{|V|} \exp\left(\frac{\sum_{j=1}^{S} \theta(j,m) \chi(j,m,k)}{\sum_{j=1}^{S} \theta(j,m)}\right)\right),$$

where

$$\begin{split} \theta(j,m) &\triangleq \exp\left(\frac{e_j^\top (\overline{X}C+P) W^{KQ}(c_{|V|+1}+P^\top e_m)}{\sqrt{d_w}}\right),\\ \chi(j,m,k) &\triangleq \left(W^{LOV} (\overline{X}C+P)^\top e_j + g + D e_m\right)_k, \end{split}$$

and $g \in \mathbb{R}^{|V|}$, $D \in \mathbb{R}^{|V| \times S}$, $W^{LOV} \in \mathbb{R}^{|V| \times p}$, $W^{KQ} \in \mathbb{R}^{p \times p}$, and $e_j \in \{0, 1\}^S$ denotes a zero vector with 1 on the *j*-th entry. (The proof is in Appendix C.)

Lemma 1 performs a reparameterization over the weight matrices W^V, W^Q, W^K, W^O , arriving at an explicit form of the MLM objective with only two weight matrices W^{KQ}, W^{LOV} . In particular, $g = W^{\ell}c_{|V|+1}, D = W^{\ell}P^{\top}, W^{LOV} = W^{\ell}(W^O)^{\top}W^V$, and $W^{KQ} = (W^K)^{\top}W^Q$ for some weight matrix W^{ℓ} . Lemma 1 also reveals two key components of the MLM objective: $\theta(j, m)$, the attention weight of token in the *m*-th position on token in the *j*-th position, and $\chi(j, m, \cdot)$, the similarity between token in the *m*-th position and token in the *j*-th position. These quantities will play a key role in facilitating the statistical interpretation of bidirectional attention.

2.2 Bidirectional attention as a mixture of continuous word experts

Building on the derivations in Lemma 1, we next establish the equivalence between the loss objective of bidirectional attention and that of the continuous bag of words (CBOW) model with mixture-of-experts (MOE) weights. This equivalence will enable us to interpret bidirectional attention as fitting a statistical model of CBOW+MOE.

The continuous bag of words model (CBOW). We begin with reviewing the CBOW formulation of word2vec [Mikolov et al., 2013]. CBOW aims to predict the center token based on the surrounding tokens (a.k.a. context tokens). It has two parameter matrices, representing the center and context embeddings respectively.

In more detail, we consider an input-output pair $(\overline{X}, \overline{y})$ as in Section 2.1, where $m \in [S]$ and $b \in [|V|]$ represent the masked position and masked token. We note that, while masking is never employed in CBOW, introducing masking into CBOW does not change its objective. The reason is that the context of a token in CBOW does not include the token itself. Thus, with window size w, the loss objective for predicting the token in the m-th position of CBOW (a.k.a. the negative log-likelihood) is

$$L_{\rm cbow}(m,b) = -\frac{\sum_{j=1}^{S} \omega(j,m)\xi(j,b)}{\sum_{j=1}^{S} \omega(j,m)} + \log\left(\sum_{k=1}^{|V|} \exp\left(\frac{\sum_{j=1}^{S} \omega(j,m)\xi(j,k)}{\sum_{j=1}^{S} \omega(j,m)}\right)\right),$$

where

$$\omega(j,m) \triangleq \mathbb{1}(1 \le |j-m| \le w),$$

$$\xi(j,k) \triangleq \left(W^{LOV}(\overline{X}C)^{\top} e_j\right)_k,$$

if we denote the center and context embedding matrices by W^{LOV} and C to match the notations of bidirectional attention.

Weight and similarity matrices in CBOW and bidirectional attention. The CBOW model appears to be related to bidirectional attention: it admits natural notions of (attention) weight and (token) similarity as in bidirectional attention. Specifically, the weight of the token in position $j \in [S]$ is determined by the distance between j and m and the number of integers between m - w and m + w (inclusive) that are within the range [1, S]. The similarity of token $\alpha \in [|V|]$ in the center and token $\beta \in [|V|]$ in the context is $(W_{\alpha}^{LOV})^{\top}c_{\beta}$, regardless of their positions in the sentence.

To compare CBOW and bidirectional attention, we next inspect the weight matrices in the MLM objective of bidirectional attention. Specifically, the weight of the token in the *j*-th position in L_{MLM} is given by²

$$\frac{\exp\left(e_j^{\top}(\overline{X}C+P)W^{KQ}(c_{|V|+1}+P^{\top}e_m)/\sqrt{d_w}\right)}{\sum_{j=1}^{S}\exp\left(e_j^{\top}(\overline{X}C+P)W^{KQ}(c_{|V|+1}+P^{\top}e_m)/\sqrt{d_w}\right)}.$$

Unlike that of CBOW, this weight matrix of bidirectional attention depends on all tokens in the masked sentence and their corresponding positions. Yet, it does not depend on the center (masked) token *b*. Further, the term inside the $\exp(\cdot)$ can be decomposed into four components:

- 1. $e_j^{\top} \overline{X} C W^{KQ} c_{|V|+1} / \sqrt{d_w}$, which depends only on the token in position *j*;
- 2. $e_j^{\top} \overline{X} C W^{KQ} P^{\top} e_m / \sqrt{d_w}$, which depends on the token in position *j*, and position *m*;
- 3. $e_j^{\top} P W^{KQ} c_{|V|+1} / \sqrt{d_w}$, which depends only on position *j*;
- 4. $e_i^{\top} P W^{KQ} P^{\top} e_m / \sqrt{d_w}$, which depends on both position j and position m.

The similarity matrix of bidirectional attention also appears to be related to that of CBOW. In bidirectional attention, the similarity of token α in the center (in position *m*) and token β in the context (in position *j*) is given by $(W_{\alpha}^{LOV})^{\top}c_{\beta} + (W_{\alpha}^{LOV})^{\top}P^{\top}e_{j} + g_{\alpha} + (D_{\alpha})^{\top}e_{m}$, which also contains four components. Moreover, the first component coincides with the similarity matrix of CBOW.

Bidirectional attention as a mixture of continuous word experts. Following these observations that bidirectional attention appears to be closely related to CBOW, we conclude this section with Theorem 2: it proves that the MLM objective of bidirectional attention in Lemma 1 is equivalent to the CBOW objective with MOE weights, where the token in each position serves as an expert.

²The weight and similarity matrices can take other parametric forms; e.g., Sonkar et al. [2020] uses a different weight function that depends on the center token b in their attention word embedding (AWE) model.

Theorem 2 (Bidirectional attention as a mixture of continuous word experts). The MLM objective of bidirectional attention is equivalent to the cross-entropy loss between the token being masked \overline{y} and the prediction probabilities softmax $(F(\overline{X}))$ from a mixture-of-experts (MOE) predictor:

$$F(\overline{X}) = \sum_{j \in [S]} \pi_j(\overline{X}) f_j(\overline{X})$$

where the *j*th expert $f_i(\overline{X})$ relies on the embedding of the token in position *j*,

$$f_j(\overline{X}) = W^{LOV}(\overline{X}C + P)^{\top}e_j + g + De_m,$$

and its weight (namely the contribution of expert j to the prediction) is $\pi_j(\overline{X}) = (\operatorname{softmax}(h(\overline{X})))_j$ with

$$h_j(\overline{X}) = e_j^{\top}(\overline{X}C + P)W^{KQ}(c_{|V|+1} + P^{\top}e_m)/\sqrt{d_w}.$$

Theorem 2 is an immediate consequence of Lemma 1. It formally establishes the equivalence between bidirectional attention and CBOW+MOE, enabling a statistical interpretation of bidirectional attention. In particular, Theorem 2 reveals the distinct use of MOE, a machine learning technique that excels at handling heterogeneous data, in bidirectional attention. This observation partially explain the empirical effectiveness of attention-based models in capturing heterogeneous patterns in complex natural language data [Devlin et al., 2019, Liu et al., 2019]. Moreover, the form of $h_j(\overline{X})$ bears resemblance to a kernel smoother in the sense that it is roughly a weighted inner product between the *j*-th token and all other tokens within the sentence.

Extensions to multi-head and multi-layer bidirectional attention. We finally extend Theorem 2 to multi-head and multi-layer bidirectional attention. For bidirectional attention with multiple attention heads, its MLM objective can be shown to be equivalent to a stacked MOE of CBOW. For example, for bidirectional attention with two attention heads, its MLM objective is equivalent to cross entropy loss with the following stacked MOE predictor:

$$F(\overline{X}) = \sum_{j \in [S]} \pi_j^1(\overline{X}) f_j^1(\overline{X}) + \sum_{j \in [S]} \pi_j^2(\overline{X}) f_j^2(\overline{X}),$$

where the *j*th expert of the *i*th head is

$$f_j^i(\overline{X}) = W^{LOV_i}(\overline{X}C + P)^{\top}e_j + \frac{g}{2} + \frac{De_m}{2}$$

and the corresponding MOE weight is $\pi_i^i(\overline{X}) = (\operatorname{softmax}(h^i(\overline{X})))_i$, with

$$h_j^i(\overline{X}) = e_j^\top (\overline{X}C + P) W^{KQ_i}(c_{|V|+1} + P^\top e_m) / \sqrt{d_w}.$$

Following similar derivations, one can show that bidirectional attention with multiple attention layers is equivalent to a mixture of MOES, i.e., a deep CBOW model with weights determined by MOES.

3 Bidirectional attention for tabular data

The equivalence between MLM with self-attention and CBOW with MOE weights (Theorem 2) suggests an immediate extension to categorical tabular data, as developed in this section. Across empirical studies, we find that this tabular extension of attention achieves significant improvement in OOD generalization over existing methods, including existing algorithms for tabular data (e.g., random forest and gradient boosting) and existing tabular generalizations of attention modules (e.g., TabTransformer and FTTransformer).

3.1 Tabular extension of bidirectional attention

To extend bidirectional attention to tabular data, we consider a classification problem with categorical features. For simplicity, we assume the response variable Y_i is ordinal with C classes. Further assume each of the K-dimensional features X_i is also ordinal with C classes. The training data contains pairs of features and responses (X_i, Y_i) . The goal is to predict the response for some test data point X.

Extending bidirectional attention to this tabular setting requires that we handle tabular features with bidirectional attention. To this end, we leverage the observation in Theorem 2 that bidirectional attention can be viewed as MOE with the token in each position (endowed with positional encodings) serving as an expert. This MOE perspective of bidirectional attention immediately suggests that we consider each tabular feature as an expert, since each position in a sentence can be viewed as a tabular feature for predicting the masked token. To summarize, one can use tabular feature encodings in place of positional encodings for analyzing tabular data with bidirectional attention.

To operationalize this idea, we first introduce "word" embeddings $w_1, \dots, w_C \in \mathbb{R}^d$ for each class and w_0 for the [MASK] token. We then introduce "position" encodings $p_1, \dots, p_{K+1} \in \mathbb{R}^d$, one for each feature. Finally, we consider the concatenation of features and covariates (X_i, Y_i) of each data point as a sentence in bidirectional attention. In order to learn the word embeddings and positional encodings using the MLM objective, we do the following:

- 1. Replace each position with the [MASK] token, one at a time.
- 2. For each masking instance, compute the sum of the corresponding word embeddings and positional encodings, and employ the usual cross-entropy loss to predict the masked token.
- 3. At test time, given a test data point X_{test} , use the trained model to predict the most probable class for the input (X_{test} , [MASK]).

We note that this use of MLM objective for tabular data implicitly models the joint distribution p(X, Y), as opposed to the conditional distribution p(Y|X) that standard supervised algorithms commonly model. As a consequence, tabular extensions of bidirectional attention can potentially achieve better ood generalization, as we demonstrate empirically next.

Finally, this tabular extension of bidirectional attention can be applied beyond supervised classification. It readily extends to unsupervised settings (if we ignore the Y_i 's) and semi-supervised settings (if we consider both the labeled and unlabeled data and set the Y_i 's for the unlabeled

Param. \setminus Acc.	LR	RF	GB	MLP	ATN
(1, 0, 0.1)	0.388	0.409	0.413	0.323	0.404
(1, 0, 0.9)	0.313	0.298	0.350	0.237	0.389
(1, 0.5, 0.1)	0.345	0.361	0.366	0.292	0.359
(1, 0.5, 0.9)	0.270	0.253	0.299	0.202	0.306
(1, 1.5, 0.1)	0.250	0.243	0.253	0.204	0.252
(1, 1.5, 0.9)	0.169	0.158	0.172	0.142	0.170
(5, 0, 0.1)	0.250	0.207	0.244	0.306	0.419
(5, 0, 0.9)	0.162	0.150	0.156	0.169	0.392
(5, 0.5, 0.1)	0.227	0.173	0.214	0.252	0.318
$\left(5, 0.5, 0.9\right)$	0.154	0.133	0.153	0.151	0.269
(5, 1.5, 0.1)	0.167	0.099	0.157	0.165	0.171
(5, 1.5, 0.9)	0.125	0.108	0.114	0.118	0.133
	(a) Accura	су		
Param. \ MSE	LR	RF	GB	MLP	ATN
(1, 0, 0.1)	3.015	2.694	2.730	4.059	2.941
(1, 0, 0.9)	5.163	9.331	4.855	7.911	3.078
(1, 0.5, 0.1)	3.416	3.201	3.123	4.704	3.281
(1, 0.5, 0.9)	5.955	10.106	6.070	8.123	4.465
(1, 1.5, 0.1)	5.725	5.685	5.415	7.199	5.594
(1, 1.5, 0.9)	8.942	12.340	9.837	9.874	7.339
(5, 0, 0.1)	5.333	8.498	5.967	2.814	1.521
(5, 0, 0.9)	5.674	10.101	8.858	7.842	1.633
(5, 0.5, 0.1)	6.021	10.236	6.844	4.056	2.605
$\left(5, 0.5, 0.9\right)$	6.118	10.427	8.283	7.884	2.355
(5, 1.5, 0.1)	9.159	16.154	9.538	8.313	8.316
(5, 1.5, 0.9)	8.410	10.409	10.110	9.966	6.501
		(b) MSE			

Table 1: The proposed tabular extension of bidirectional attention (ATN) achieves better or competitive accuracy and MSE than competing methods, across all parameter settings. The parameter tuples indicate different choices of $(n_c, \text{noise}, \text{corr})$.

data to be [MASK]). This approach is also applicable to multiple data sets with only partially overlapping features: the learned feature encodings will allow us to bring all features into the same embedding space. These learned encodings can also reveal the relationships between different tabular features across different data sets.

3.2 Empirical studies of tabular bidirectional attention

In this section, we empirically study the tabular extension of bidirectional attention using simulated and real data sets. Across empirical studies, we find that this approach outperforms in OOD generalization for tabular data, as compared with both existing tabular data algorithms and existing tabular extensions of attention modules.

3.2.1 Simulated data

We begin with evaluating tabular bidirectional attention on simulated data. We focus on the common OOD generalization setting of covariate shift; it refers to prediction tasks where $p(X_{\text{train}}) \neq p(X_{\text{test}})$ and $p(Y_{\text{train}}|X_{\text{train}}) = p(Y_{\text{test}}|X_{\text{test}})$.

Data generation. We describe the key components of the data generation process; we refer the readers to Appendix D for full details. We set the number of features K to be 5, the number of classes C to be 10, and both the training and test set size to be 2,000. Twenty data sets are generated for each combination of hyperparameters.

Competing methods and evaluation metrics. We fit the proposed tabular extension of bidirectional attention model to each training set, together with a few competing methods, namely logistic regression (LR), random forests (RF), gradient boosting (GB) and multilayer perceptron (MLP). See Appendix E for implementation details.

Results. Section 3.1 summarizes the test accuracy and mean squared error of all methods. We find that the proposed tabular extension of bidirectional attention outperforms or competitively compares to all competing methods. Moreover, its performance gain is more apparent when corr = 0.9 (very correlated training features) as compared to when corr = 0.1; the former corresponds to a more challenging case of covariate shift.

3.2.2 UCI's auto-mpg data

We next study the tabular extension of bidirectional attention on a real data set, namely the auto-mpg data from the UCI data set. This data set contains the following information from 398 different car models: *mpg*, *cylinders*, *displacement*, *horsepower*, *weight*, *acceleration*, *model year*, *origin*, and *car name*.

Data processing. To simulate covariate shift, we follow the approach of Sugiyama and Storkey [2006]: we assigns cars from origin 1 to the training set, and origins 2 and 3 to the test set. In addition, we only consider cars with 4, 6 or 8 cylinders and remove data points with missing values. Lastly, similar to the synthetic data experiments, we convert each column into three quantile-based categories. The final data set has 385 data points, where 245 belong to the training set and 140 belong to the test set.

	LR	RF	GB	MLP	CE	FT	TT	AI	TN	ATN (ours)
Accuracy	0.657	0.721	0.657	0.700	0.764	0.707	0.707	0.364	0.600	0.793
MSE	0.343	0.279	0.343	0.300	0.236	0.293	0.293	0.636	0.486	0.207

Table 2: The proposed tabular extension of attention (ATN) achieves superior performance as compared to all baselines. (Lower MSE and higher accuracy is better.)

Competing methods and evaluation metrics. We use the same competing methods and evaluation metrics as in Section 3.2.1. Additionally, we compare with other existing tabular extensions of attention modules, including CategoryEmbedding (CE) [Joseph, 2021], FTTransformer (FT) [Gorishniy et al., 2021], TabTransformer (TT) [Huang et al., 2020], AutoInt (AI) [Song et al., 2019], and TabNet (TN) [Arik and Pfister, 2021].³

Results. Section 3.2.2 summarizes the test accuracy and mean squared error of all methods. We find that the proposed tabular extension of bidirectional attention outperforms all competing methods. This performance gain is likely due to its focus on modeling the joint distribution of the covariates and response variable; it is in contrast to the practice of modeling only the conditional distribution of the response variable given the covariates in supervised learning.

4 Linear word analogies in attention-based embeddings

In this section, we explore the presence of linear word analogies in the embeddings of bidirectional attention and its non-attention predecessors. En route, we leverage the close connection between CBOW and bidirectional attention in Theorem 2 to facilitate the theoretical analysis. This exploration is motivated by a curious empirical observation: While bidirectional attention (e.g., BERT) often significantly outperforms its non-attention predecessors in natural language processing benchmarks, it does not seem to outperform its predecessors in word analogy tasks. In particular, it can sometimes perform worse as compared to classical word embedding algorithms like word2vec [Mikolov et al., 2013] and GloVe [Pennington et al., 2014].

Thanks to these empirical observations, we characterize under which conditions bidirectional attention and CBOW can exhibit linear word analogies in their embeddings. We find that bidirectional attention requires much stronger conditions to exhibit linear word analogies than its non-attention predecessors. These results partially explain the limited empirical gain in using bidirectional attention for word analogy tasks.

4.1 A curious empirical study: Do attention-based token embeddings exhibit linear word analogies?

We begin with a curious empirical study about the presence of linear word analogies in attentionbased and non-attention-based token embeddings. Linear structure in neural word embeddings such as word2vec [Mikolov et al., 2013] and GloVe [Pennington et al., 2014] is a well-known

³We use pytorch_tabular's [Joseph, 2021] implementation with the default parameters. The batch and epoch sizes are set to be 128 and 200, respectively.

Accuracy	BERT	GloVe	CBOW	Cosine similarity	BERT	GloVe	CBOV
Semantic	0.641	0.759	0.234	Semantic	0.500	0.600	0.504
Syntactic	0.754	0.692	0.667	Syntactic	0.610	0.610	0.582
Overall	0.727	0.708	0.563	Overall	0.584	0.607	0.564

Table 3: Classical word embedding methods can achieve similar or higher performance than attention-based model in word analogy tasks: GloVe achieve higher or the same average cosine similarity than BERT on both syntactic and semantic analogies; GloVe also outperforms BERT in accuracy for semantic analogies. (Higher is better.)

empirical phenomenon. However, most studies focused on embeddings trained via SGNS [Allen and Hospedales, 2019, Ethayarajh et al., 2019]. This phenomenon is less studied in other language modeling approaches, e.g., CBOW and bidirectional attention, with few exceptions [Ushio et al., 2021].

To this end, we first perform an empirical study about whether linear relationships are observed in embeddings from word2vec trained with the CBOW objective and BERT [Devlin et al., 2019], a large language model based on bidirectional attention. Following existing studies, we use the analogy identification task as a proxy for identifying the presence of linear relationships, utilizing the analogy data set first introduced in Pennington et al. [2014]. We refer the readers to Appendix F for data set and implementation details.

Evaluation metrics. For each model, we are interested in (1) the overall and per-category accuracies, where accuracy is defined as the proportion of correct answers; and (2) the overall and per-category average cosine similarity between $x_b + x_c - x_a$ and the correct answer. We note that (2) is a better metric than (1) due to the difference in vocabulary sizes across models.

Results. The accuracy and average cosine similarity for each model is displayed in Section 4.1. We observe that all three models generally result in word embeddings that exhibit certain degrees of linear word analogies. However, the bidirectional attention model BERT can often perform worse than its non-attention predecessor GloVe in this task, despite it being a much more powerful language model as evidenced by its performance in common natural language benchmarks.

What factors have limited BERT's (and bidirectional attention's) ability to exhibit linear word analogies? What about CBOW and GloVe? Below we study these questions theoretically, leveraging the close connection between CBOW and bidirectional attention in Theorem 2. In particular, we characterize the conditions under which CBOW and bidirectional attention may exhibit linear word analogies. We find that the conditions required by bidirectional attention are much stronger, which partially explains the empirical observations above.

4.2 Linear word analogies in CBOW and bidirectional attention embeddings

We begin with theoretically characterizing under which conditions CBOW embeddings can exhibit linear word analogies. Starting with Allen and Hospedales's [2019] argument for SGNS, we extend the argument to both CBOW and attention-based token embeddings, thanks to the equivalence we established in Theorem 2.

To perform this theoretical analysis, we follow existing analyses about sGNS: Levy and Goldberg [2014] showed that for a sufficiently large embedding dimension, embeddings from sGNS satisfy $w_i^{\top}c_j = \log\left(\frac{p(w_i,c_j)}{p(w_i)p(c_j)}\right) - \log k = \text{PMI}(w_i,c_j) - \log k$, where k is the number of negative samples for each positive sample; $W^{LOV}, C \in \mathbb{R}^{|V| \times p}$ are the center and context embedding matrix, respectively. For each $i \in [|V|], w_i^{\top}(c_i^{\top})$ is the *i*-th row of W^{LOV} (C), which represents the center (context) embedding of word *i*.

Using this result, Allen and Hospedales [2019] considered embeddings which factorize the unshifted PMI matrix, namely $w_i^{\top}c_j = PMI(w_i, c_j)$, compactly written as $W^{\top}C = PMI$. Through the ideas of *paraphrases* and *word transformations*, they explained why linear relationships exist for analogies on SGNS word embeddings.

Here, we perform similar analyses for CBOW and bidirectional attention; the goal is to characterize the conditions under which CBOW and bidirectional attention can exhibit linear word analogies respectively. Below we sketch the main results we obtain, deferring full details to Appendix G.

Linear word analogies in CBOW embeddings. We first characterize the inner product of center and context embeddings of CBOW.

Proposition 3. Embeddings from fitting CBOW without negative sampling must satisfy $w_i^{\top} c_j \approx \log\left(\frac{p(w_i,c_j)}{p(c_j)}\right) + \log |V|.$

This result suggests that CBOW approximately factorizes M, a $|V| \times |V|$ matrix such that $M_{i,j} = \log\left(\frac{p(w_i,c_j)}{p(c_j)}\right) + \log|V|$. Following this result, we next argue that the CBOW embeddings approximately form a linear relationship, up to some error terms.

Proposition 4. Given any $w_a, w_{a^*}, w_b, w_{b^*} \in \mathcal{E}$, we have

$$w_{b^*} = w_{a^*} - w_a + w_b + C^{\dagger}(\rho^{\mathcal{W},\mathcal{W}_*} + \Delta^{\mathcal{W},\mathcal{W}_*} + \delta^{\mathcal{W},\mathcal{W}_*})$$
$$= w_{a^*} - w_a + w_b + C^{\dagger}(\xi^{\mathcal{W},\mathcal{W}_*} + \Delta^{\mathcal{W},\mathcal{W}_*}),$$

where \mathcal{E} is the set of all words in the vocabulary, $\mathcal{W} = \{w_b, w_{a^*}\}, \Delta^{\mathcal{W},\mathcal{W}_*} = \sigma^{\mathcal{W}} - \sigma^{\mathcal{W}_*}$ and $\mathcal{W}_* = \{w_{b^*}, w_a\}$. The quantities $\rho^{\mathcal{W},\mathcal{W}_*}, \Delta^{\mathcal{W},\mathcal{W}_*}, \delta^{\mathcal{W},\mathcal{W}_*}, \xi^{\mathcal{W},\mathcal{W}_*}$ are all statistics that characterize the relationships between the two word sets $\mathcal{W}, \mathcal{W}_*$. We refer the reader to Appendix G for their precise definitions and complete details of the results.

Proposition 4 reveals that we have linear word analogies $w_{b^*} \approx w_{a^*} - w_a + w_b$ when \mathcal{W} paraphrases \mathcal{W}_* in the sense of Allen and Hospedales [2019] (i.e. $\rho^{\mathcal{W},\mathcal{W}_*} \approx 0$), and $\sigma^{\mathcal{W}}, \sigma^{\mathcal{W}_*}$ and $\delta^{\mathcal{W},\mathcal{W}_*}$ are small. The latter conditions hold true only when all $w_i \in \mathcal{W}$ ($w_i \in \mathcal{W}_*$) are approximately

conditionally independent given c_j , and $p(W) \approx p(W_*)$. If we consider alternative definitions of paraphrase—which we detail in Appendix G, then the linear analogy error may only depend on the approximate conditional independence of w_i 's given c_j .

Finally, we characterize the conditions under which, if token embeddings of CBOW exhibit linear word analogies, then its contextual embedding will also exhibit this structure.

Proposition 5. Let $\mathcal{W} = \{r, s\}$ and $\mathcal{W}_* = \{t, u\}$. Assume $p(\mathcal{W}) \approx p(\mathcal{W}_*)$ and $w_i \in \mathcal{W}$ $(w_i \in \mathcal{W}_*)$ are approximately marginally independent. Further, assume that W has full row rank. If $w_r + w_s \approx w_t + w_u$, then $c_r + c_s \approx c_t + c_u$.

Linear word analogies for bidirectional attention. We next extend these CBOW arguments to bidirectional attention, leveraging the close connection established in Theorem 2. We will show that the same linear word analogies may emerge in bidirectional attention, but under much stronger assumptions.

Proposition 6. Token embeddings from bidirectional attention must satisfy

$$w_i^{\top} c_j \approx \frac{|V| \sum_{(i,j)} \gamma_j^i - \left(\sum_{(1,j)} \gamma_j^1 + \dots + \sum_{(|V|,j)} \gamma_j^{|V|} \right)}{S\left(\sum_{(1,j)} (\gamma_j^1)^2 + \dots + \sum_{(|V|,j)} (\gamma_j^{|V|})^2 \right)},$$

where for a center-context pair (d, j) in the masked sentence (a_1, \dots, a_S) , we define $\gamma_j^d = \tau_j / \sum_{s=1}^S \tau_{a_s}$, and $\tau_j = \exp\left(c_j^\top W^{KQ} c_{|V|+1} / \sqrt{d_w}\right)$.

Proposition 6 shows that bidirectional attention approximately factorizes a $|V| \times |V|$ matrix whose (i, j)-th entry is given by the equation above. Unlike in CBOW, the token embedding for each word i is c_i (the *context* embedding), and not w_i (the *center* embedding). In the case where τ_j is approximately the same for every $j \in [|V| + 1]$, the problem approximately reduces to a vanilla CBOW: we always have $\gamma_j^d \approx 1/S$, whence Proposition 6 yields $w_i^\top c_j \approx \frac{p(w_i, c_j)}{p(c_j)} \cdot |V| - 1 \approx \log\left(\frac{p(w_i, c_j)}{p(c_i)}\right) + \log |V|$.

Following a similar argument as Proposition 4, we argue that the bidirectional attention embedding can also exhibit linear word analogies, up to some error.

Proposition 7. Given any $w_a, w_{a^*}, w_b, w_{b^*} \in \mathcal{E}$, we have

$$w_{b^*} = w_{a^*} - w_a + w_b + \tilde{C}^{\dagger}(\bar{\rho}^{\mathcal{W},\mathcal{W}_*} + \overline{\Delta}^{\mathcal{W},\mathcal{W}_*} + \bar{\delta}^{\mathcal{W},\mathcal{W}_*})$$
$$= w_{a^*} - w_a + w_b + \tilde{C}^{\dagger}(\bar{\xi}^{\mathcal{W},\mathcal{W}_*} + \overline{\Delta}^{\mathcal{W},\mathcal{W}_*}),$$

where $\overline{\Delta}^{W,W_*} = \overline{\sigma}^W - \overline{\sigma}^{W_*}$, $W = \{w_b, w_{a^*}\}$, and $W_* = \{w_{b^*}, w_a\}$. The quantities $\overline{\rho}^{W,W_*}, \overline{\Delta}^{WW_*}$, $\overline{\delta}^{W,W_*}$ characterize the relationships between W, W_* based on $\overline{p}(w_i, c_j) \triangleq \sum_{(i,j)} \gamma_j^i / E$; see details in Appendix G.

Under additional conditions, similar linear word analogy relationships may also emerge for the contextual embeddings of bidirectional attention.

Proposition 8. Let $\mathcal{W} = \{r, s\}$ and $\mathcal{W}_* = \{t, u\}$. Assume $\bar{p}(\mathcal{W}) \approx \bar{p}(\mathcal{W}_*)$ and $w_i \in \mathcal{W}$ $(w_i \in \mathcal{W}_*)$ are approximately marginally independent. Further assume that W has full row rank and $\bar{p}(w_i, c_j) \approx \bar{p}(w_j, c_i)$. If $w_r + w_s \approx w_t + w_u$, then $\tilde{c}_r + \tilde{c}_s \approx \tilde{c}_t + \tilde{c}_u$.

While we leave the full details of these results to Appendix G, Propositions 7 and 8 suggest that bidirectional attention requires much stronger conditions to exhibit linear relationships than CBOW. Specifically, it requires the quantity $\bar{p}(w_i, c_j) = \sum_{(i,j)} \gamma_j^i / E$ to be approximately symmetric. Even when this condition holds, linear word analogy would only hold for some transformed embeddings \tilde{c}_i 's, as opposed to the token embeddings c_i 's. Only under an additional assumption that $\zeta_j := \frac{\sum_{(1,j)} (\gamma_j^1)^2 + \dots + \sum_{(|V|,j)} (\gamma_j^{|V|})^2}{\sum_{(1,j)} \gamma_j^1 + \dots + \sum_{(|V|,j)} \gamma_j^{|V|}}$ is approximately the same for each j (e.g., when τ_j is approximately the same for every j) will we approximately have linear word analogies for the token embeddings c_i 's.

Finally, we note that all these results can be easily extended to incorporate positional encodings by considering each (word, position) pair as a unit. In these cases, analogies will be drawn between (word, position) pairs.

5 Discussion

In this paper, we prove that a single-head single-layer bidirectional attention is equivalent to a continuous bag of words (CBOW) model with mixture-of-experts (MOE) weights, upon reparameterization. This statistical perspective reveals the distinct use of MOE in bidirectional attention, supporting the empirical observation that bidirectional attention excels in capturing heterogeneous patterns. This connection further suggests immediate extensions of bidirectional attention to tabular data, leading to improved out-of-distribution (OOD) generalizations when compared to existing approaches. It also allows us to characterize the conditions under which embeddings from bidirectional attention and CBOW exhibit linear word analogies. These analyses show that bidirectional attention requires much stronger assumptions than its non-attention predecessors to exhibit linear word analogies.

One limitation of this work is that the linear word analogy argument in Section 4 ignores residual connections. In addition, we only consider bidirectional attention architectures that use linear layers, as opposed to feed-forward layers used in Devlin et al. [2019]. Beyond addressing these limitations, exploring the statistical properties of bidirectional attention is an interesting avenue for future work. It will also be useful to provide theoretical justifications for the observed robustness of bidirectional attention to covariate shifts, and to understand the fundamental differences between static and contextual word embeddings in their abilities to form linear analogies.

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Supplementary Material: Bidirectional Attention as a Mixture of Continuous Word Experts

A Summary of notations

Below is a summary of commonly-used notations in Section 4.

Notation	Explanation
V	Vocabulary size
S	Sentence length
p	Embedding dimension
W^{LOV}	Center embedding matrix
C	Token (context) embedding matrix
w_i^{\top}	i -th row of W^{LOV}
c_i^{\top}	i-th row of C
P	Position encoding matrix
\overline{X}	One-hot encoding matrix of the masked sentence
\overline{y}	One-hot encoding of the target word
m	Position of the masked word
b	The masked word
e_j	A zero vector of length S with 1 on the j -th entry
$f_j(\cdot)$	The output generated by expert j
$\pi_j(\cdot)$	The contribution of expert j
a_s	The word on the <i>s</i> -th position of the masked sentence

B A sketch of the attention-based architecture

- 1. Let $X = \overline{X}C \in \mathbb{R}^{S \times p}$ be a matrix consisting of the token embeddings of each word in the masked sentence, and $X' = X + P \in \mathbb{R}^{S \times p}$.
- 2. Introduce attention weight matrices $W^V \in \mathbb{R}^{d \times p}$, $W^Q \in \mathbb{R}^{d_w \times p}$ and $W^K \in \mathbb{R}^{d_w \times p}$. Let $X^{\text{attn}} = \text{softmax}\left(\frac{X'(W^Q)^\top W^K(X')^\top}{\sqrt{d_w}}\right) X'(W^V)^\top \in \mathbb{R}^{S \times d}$, where the softmax is taken row-wise.
- 3. Let $W^O \in \mathbb{R}^{d \times p}$, and write $Z = X^{\operatorname{attn}} W^O \in \mathbb{R}^{S \times p}$.
- 4. Introduce a residual connection, and write $Z' := X' + Z \in \mathbb{R}^{S \times p}$.
- 5. For each position $i \in [S]$, apply a linear layer $LIN_1(Z'_i) = W'Z'_i \in \mathbb{R}^p$, where $W' \in \mathbb{R}^{p \times p}$.
- 6. Introduce another residual connection, and write $Z'' = Z' + LIN_1(Z') \in \mathbb{R}^{S \times p}$.
- 7. For each position $i \in [S]$, apply a linear layer $LIN_2(Z''_i) := W''Z''_i \in \mathbb{R}^{|V|}$, where $W'' \in \mathbb{R}^{|V| \times p}$.

8. Perform the softmax operation and calculate the cross-entropy loss corresponding to predicting the masked word in the sentence.

C Proof of Lemma 1

Proof. Recall that $m \in [S]$ and $b \in [|V|]$ represent the masked position and masked word, respectively. It is easy to see that $X^{\top}e_m = c_{|V|+1}$, where $e_m \in \{0, 1\}^S$ is a zero vector with 1 on the *m*-th entry. Note that steps 1 to 4 of Appendix B give us

$$Z' = X + P + \operatorname{softmax}\left(\frac{(X+P)(W^Q)^\top W^K (X+P)^\top}{\sqrt{d_w}}\right) (X+P)(W^V)^\top W^O \in \mathbb{R}^{S \times p}.$$

This is followed by steps 5 and 6, which yield $Z'' = Z' + LIN_1(Z')$ where the *i*-th row of Z'' is given by $(Z''_i)^{\top}$, where $Z''_i = Z'_i + W'Z'_i$ for some $W' \in \mathbb{R}^{p \times p}$. Lastly, steps 7 and 8 result in $\alpha_m = \operatorname{softmax}(W''Z''_m)$ for some $W'' \in \mathbb{R}^{|V| \times p}$, from which the loss is simply $-\log(e_b^{\top}\alpha_m)$, where $e_b \in \{0, 1\}^{|V|}$ is a zero vector with 1 on the *b*-th entry. See that

$$\begin{split} W''Z''_m \\ &= (W'' + W''W')(Z')^\top e_m \\ &= W^\ell \left((X+P)^\top + (W^O)^\top W^V (X+P)^\top \operatorname{softmax} \left(\frac{(X+P)(W^K)^\top W^Q (X+P)^\top}{\sqrt{d_w}} \right) \right) e_m, \end{split}$$

where $W^{\ell} = W'' + W''W' \in \mathbb{R}^{|V| \times p}$ and the softmax is taken column-wise. Writing $W^{\ell}c_{|V|+1} = g \in \mathbb{R}^{|V|}$, $W^{\ell}P^{\top} = D \in \mathbb{R}^{|V| \times S}$, $W^{\ell}(W^{O})^{\top}W^{V} = W^{LOV} \in \mathbb{R}^{|V| \times p}$ and $(W^{K})^{\top}W^{Q} = W^{KQ} \in \mathbb{R}^{p \times p}$, we obtain

$$W''Z''_{m} = g + De_{m} + \sum_{j=1}^{S} \frac{\exp\left(\frac{e_{j}^{\top}(X+P)W^{KQ}(c_{|V|+1}+P^{\top}e_{m})}{\sqrt{d_{w}}}\right)}{\sum_{j=1}^{S}\exp\left(\frac{e_{j}^{\top}(X+P)W^{KQ}(c_{|V|+1}+P^{\top}e_{m})}{\sqrt{d_{w}}}\right)} \left(W^{LOV}(X+P)^{\top}e_{j}\right)$$
$$= \sum_{j=1}^{S} \frac{\exp\left(\frac{e_{j}^{\top}(\overline{X}C+P)W^{KQ}(c_{|V|+1}+P^{\top}e_{m})}{\sqrt{d_{w}}}\right)}{\sum_{j=1}^{S}\exp\left(\frac{e_{j}^{\top}(\overline{X}C+P)W^{KQ}(c_{|V|+1}+P^{\top}e_{m})}{\sqrt{d_{w}}}\right)} \left(W^{LOV}(\overline{X}C+P)^{\top}e_{j}+g+De_{m}\right) + \sum_{j=1}^{S} \frac{\exp\left(\frac{e_{j}^{\top}(\overline{X}C+P)W^{KQ}(c_{|V|+1}+P^{\top}e_{m})}{\sqrt{d_{w}}}\right)}{\sum_{j=1}^{S}\exp\left(\frac{e_{j}^{\top}(\overline{X}C+P)W^{KQ}(c_{|V|+1}+P^{\top}e_{m})}{\sqrt{d_{w}}}\right)} + \sum_{j=1}^{S} \frac{\exp\left(\frac{e_{j}^{\top}(\overline{X}C+P)W^{KQ}(c_{|V|+1}+P^{\top}e_{m})}{\sqrt{d_{w}}}\right)}{\sum_{j=1}^{S}\exp\left(\frac{e_{j}^{\top}(\overline{X}C+P)W^{KQ}(c_{|V|+1}+P^{\top}e_{m})}{\sqrt{d_{w}}}\right)} + \sum_{j=1}^{S} \frac{\exp\left(\frac{e_{j}^{\top}(\overline{X}C+P)W^{KQ}(c_{|V|+1}+P^{\top}e_{m})}{\sqrt{d_{w}}}\right)}{\sum_{j=1}^{S}\exp\left(\frac{e_{j}^{\top}(\overline{X}C+P)W^{KQ}(c_{|V|+1}+P^{\top}e_{m})}{\sqrt{d_{w}}}\right)} + \sum_{j=1}^{S} \frac{\exp\left(\frac{e_{j}^{\top}(\overline{X}C+P)W^{KQ}(c_{|V|+1}+P^{\top}e_{m})}{\sqrt{d_{w}}}\right)}{\sum_{j=1}^{S} \exp\left(\frac{e_{j}^{\top}(\overline{X}C+P)W^{KQ}(c_{|V|+1}+P^{\top}e_{m})}{\sqrt{d_{w}}}\right)} + \sum_{j=1}^{S} \frac{\exp\left(\frac{e_{j}^{\top}(\overline{X}C+P)W^{KQ}(c_{|V|+1}+P^{\top}e_{m})}{\sqrt{d_{w}}}\right)}{\sum_{j=1}^{S} \exp\left(\frac{e_{j}^{\top}(\overline{X}C+P)W^{KQ}(c_{|V|+1}+P^{\top}e_{m})}{\sqrt{d_{w}}}\right)} + \sum_{j=1}^{S} \frac{\exp\left(\frac{e_{j}^{\top}(\overline{X}C+P)W^{KQ}(c_{|V|+1}+P^{\top}e_{m})}{\sqrt{d_{w}}}\right)}{\sum_{j=1}^{S} \exp\left(\frac{e_{j}^{\top}(\overline{X}C+P)W^{KQ}(c_{|V|+1}+P^{\top}e_{m})}{\sqrt{d_{w}}}\right)} + \sum_{j=1}^{S} \frac{\exp\left(\frac{e_{j}^{\top}(\overline{X}C+P)W^{KQ}(c_{|V|+1}+P^{\top}e_{m})}{\sqrt{d_{w}}}\right)}}{\sum_{j=1}^{S} \exp\left(\frac{e_{j}^{\top}(\overline{X}C+P)W^{KQ}(c_{|V|+1}+P^{\top}e_{m})}{\sqrt{d_{w}}}\right)} + \sum_{j=1}^{S} \frac{\exp\left(\frac{e_{j}^{\top}(\overline{X}C+P)W^{KQ}(c_{|V|+1}+P^{\top}e_{m})}{\sqrt{d_{w}}}\right)} + \sum_{j=1}^{S} \frac{\exp\left(\frac{e_{j}^{\top}(\overline{X}C+P)W^{KQ}(c_{|V|+1}+P^{\top}e_{m})}{\sqrt{d_{w}}}\right)}}$$

and the objective for this particular instance is

$$-\frac{\sum_{j=1}^{S} \theta(j,m)\chi(j,m,b)}{\sum_{j=1}^{S} \theta(j,m)} + \log\left(\sum_{k=1}^{|V|} \exp\left(\frac{\sum_{j=1}^{S} \theta(j,m)\chi(j,m,k)}{\sum_{j=1}^{S} \theta(j,m)}\right)\right)$$

where

$$\theta(j,m) \triangleq \exp\left(\frac{e_j^\top (\overline{X}C+P)W^{KQ}(c_{|V|+1}+P^\top e_m)}{\sqrt{d_w}}\right),$$
$$\chi(j,m,k) \triangleq \left(W^{LOV}(\overline{X}C+P)^\top e_j + g + De_m\right)_k,$$

completing the proof.

D Tabular data generation process

We set the number of features K to be 5, the number of classes C to be 10, and the training and test set size to be 2,000 each. Twenty data sets are generated for each combination of hyperparameters: (1) $n_c \in \{1, 5\}$, the number of features which generate Y; (2) noise $\in \{0, 0.5, 1.5\}$, where a larger value indicates a larger noise in the observed features; and (3) corr $\in \{0.1, 0.9\}$, where a larger value indicates a larger between-feature correlation in the training set as compared to the test set.

To simulate covariate shift, we introduce the parameter corr: the correlation of any covariate pair is \pm corr in the training set, and 1 - corr in the test set. We generate the responses as a linear combination of the covariates. Moreover, we add Gaussian noise to the covariates, mimicking settings where covariates are measured with error. Lastly, we bin each covariate and response into C = 10 categories based on their quantiles. This results in a 10-class classification problem with ordinal covariates and responses.

For a fixed $n_c \in \{1, 5\}$, noise $\in \{0, 0.5, 1.5\}$ and corr $\in \{0.1, 0.9\}$, our data generation process can be described as follows.

- 1. Let train_cov = corr $\cdot J_5 + (1 corr) \cdot I_5$ and test_cov = $(1 corr) \cdot J_5 + corr \cdot I_5$. Here, J_5 represents a 5×5 matrix whose entries are all 1, and I_5 represents a 5×5 identity matrix.
- 2. Generate samples train_x_true and test_x_true from zero-mean multivariate normal distributions with covariance matrices train_cov and test_cov, respectively. Each sample is of size 2,000.
- 3. Introduce positively and negatively correlated covariates in the training samples by multiplying data in the first two features by -1.
- 4. Add Gaussian observation noises to the training and test samples. For the n_c features which generate the response, add $0.4 \cdot \text{noise} \cdot \mathcal{N}(0, 1)$; otherwise, add $0.3 \cdot \text{noise} \cdot \mathcal{N}(0, 1)$. Let the resulting samples be train_x and test_x.
- 5. Generate the true coefficient for each of the n_c features from $\mathcal{U}(0, 10)$.
- 6. Generate the training response train_y, which is a linear combinations of the n_c features of train_x_true with the true coefficients as weights, plus a Gaussian noise from $\mathcal{N}(0, 4)$. Generate the test response test_y in a similar manner.
- 7. Bin each feature and response of (train_x, train_y) and (test_x, test_y) into 10 quantilebased categories.

E Implementation and hyperameter tuning process for competing models

We fit the proposed tabular extension of bidirectional attention model to each training set, together with a few competing methods, namely logistic regression (LR), random forests (RF), gradient boosting (GB) and multilayer perceptron (MLP). We then evaluate the prediction accuracy (Acc) and mean squared error (MSE) on the corresponding test set. For each set of hyperparameters, we take the average of both metrics across the 20 generated data sets.

We implement the proposed extension of bidirectional attention (ATN) in Keras using a single-layer BERT [Devlin et al., 2019] with 5 heads, an embedding size of 20, and a feed-forward layer of dimension 5. We use the Adam optimizer with the default parameters, and a batch and epoch size of 128 and 200, respectively. For the competing methods, we use sklearn's implementation with hyperparameters chosen via 5-fold cross-validation in classification accuracy.

For each data set, the hyperparameters of the random forest (RF), gradient boosting (GB) and multilayer perceptron (MLP) models are chosen via 5-fold cross-validation based on the classification accuracy.

Random forest. We consider every combination of the following hyperparameters: (a) *criterion*: gini or entropy; (b) *n_estimators*: 50, 100 or 200; and (c) *max_depth*: 1, 3 or None.

Gradient boosting. We consider every combination of the following hyperparameters: (a) *learning_rate*: 0.01, 0.1 or 1; (b) *n_estimators*: 50, 100 or 200; and (c) *max_depth*: 1, 3 or 5.

Multilayer perceptron. We consider every combination of the following hyperparameters: (a) *hidden_layer_sizes*: (50,), (100,) or (100,50); (b) *alpha*: 0.0001, 0.001 or 0.01; and (c) *learning_rate*: constant or adaptive.

F Details of the word analogy experiment

Data description. We use the analogy data set first introduced in Pennington et al. [2014]. This data set contains 19,544 questions of the form "*a* is to *b* as *c* is to ?", together with the correct answers. As an example, the first question in the data set is "Athens is to Greece as Baghdad is to ?" (correct answer: Iraq). Overall, these questions can be categorized into two groups: semantic (about people and places) and syntactic (about word forms such as comparative, superlative and plural). For each question, we look for the word $d \neq a, b, c$ in the vocabulary such that the cosine similarity between x_d and $x_b + x_c - x_a$ is maximized; x_i represents the embedding of word *i*.

We only include a question when all four words involved are present in the vocabulary list of each model. Out of 19,544 questions in the data set, 9,522 (49%) of them satisfy this condition. Analyzing each category separately, we find that the condition is satisfied for 2,278 (26%) out of 8,869 semantic questions, and 7,244 (68%) out of 10,675 syntactic questions.

Models. We consider three models: (1) BERT base uncased, which is used in the original BERT paper [Devlin et al., 2019]; (2) GloVe trained on Wikipedia [Pennington et al., 2014]; (3) word2vec trained with CBOW [Mikolov et al., 2013]. The embedding dimensions of these models are 768,

300, 300 and 768, respectively, while the vocabulary size are around 30K, 400K, 3M and 30K, respectively. Since all questions in the data set consist of single words (e.g., not *golden_retriever*). In order to perform a fair comparison among these models, we only consider single words as possible answers to each question; we also exclude non-words (e.g., *[unused9]*, ## ?) from the list of possible answers.

G Detailed analysis of embeddings for своw and bidirectional attention

We begin with theoretically characterize under which conditions can CBOW embeddings exhibit linear word analogies. Adopting Allen and Hospedales's [2019] argument for skip-gram with negative sampling (SGNS), we extend the argument to both CBOW and attention-based token embeddings, thanks to the equivalence we established in Theorem 2.

G.1 Linear word analogies in CBOW embeddings

To perform this theoretical analysis, we follow existing analyses about SGNS: Levy and Goldberg [2014] showed that for a sufficiently large embedding dimension, embeddings from SGNS satisfy $w_i^{\top}c_j = \log\left(\frac{p(w_i,c_j)}{p(w_i)p(c_j)}\right) - \log k = \text{PMI}(w_i,c_j) - \log k$, where k is the number of negative samples for each positive sample; $W^{LOV}, C \in \mathbb{R}^{|V| \times p}$ are the center and context embedding matrix, respectively. For each $i \in [|V|], w_i^{\top}(c_i^{\top})$ is the *i*-th row of W^{LOV} (C), which represents the center (context) embedding of word *i*.

Using this result, Allen and Hospedales [2019] considered embeddings which factorize the unshifted PMI matrix, namely $w_i^{\top}c_j = \text{PMI}(w_i, c_j)$, compactly written as $W^{\top}C = \text{PMI}$. Through the ideas of *paraphrases* and *word transformations*, they explained why linear relationships exist for analogies on SGNS word embeddings.

We next perform similar analyses for CBOW and bidirectional attention to characterize their conditions required for linear word analogies.

What matrix does CBOW (approximately) factorize? Proposition 9 is the CBOW version of Levy and Goldberg's [2014] classical result on between-token similarities for SGNS. The proof can be found in Appendix H.

Proposition 9. Consider CBOW without negative sampling. Using the same notation as before, we have

$$w_i^{\mathsf{T}} c_j \approx \log\left(\frac{p(w_i, c_j)}{p(c_j)}\right) + \log|V|.$$

From Proposition 9, we know that CBOW approximately factorizes M, a $|V| \times |V|$ matrix such that

$$M_{i,j} = \log\left(\frac{p(w_i, c_j)}{p(c_j)}\right) + \log|V|.$$

It is worth noting that this formula is similar to that for noise-contrastive estimation (NCE) as mentioned in Levy and Goldberg [2014], with $\log |V|$ replaced by $-\log k$. Also, observe that $w_i^{\top}c_j > w_k^{\top}c_j$ if and only if $p(w_i, c_j) > p(w_k, c_j)$.

We empirically verify Proposition 9 using a toy corpus with a vocabulary size of 12. This corpus consists of 10,000 sentences, each of which has length 5. The corpus generation process is detailed in Appendix I. We then train a CBOW model with the whole sentence except the center word as the context. We choose the embedding dimension to be one of $\{30, 100, 300, 900\}$. For each dimension, we compute (1) the Spearman correlation between $w_i^{\top}c_j$ and $p(w_i, c_j)/p(c_j)$ for each i, j; and (2) the Pearson correlation between $w_i^{\top}c_j$ and $\log(p(w_i, c_j)/p(c_j)) + \log |V|$ for each i, j such that the latter is well-defined. We obtain values of (0.74, 0.77, 0.77, 0.77) for (1) and (0.67, 0.71, 0.70, 0.71) for (2), which are reasonably high.

The paraphrasing argument for CBOW. We look at what it means for two word sets to paraphrase each other.

Definition 10 (Definition D2 of Allen and Hospedales [2019]). Let \mathcal{E} be the set of all words in the vocabulary. Two word sets $\mathcal{W}, \mathcal{W}_* \subseteq \mathcal{E}$ are said to paraphrase each other if the paraphrase error $\rho^{\mathcal{W},\mathcal{W}_*} \in \mathbb{R}^{|V|}$ is element-wise small, where

$$\rho_j^{\mathcal{W},\mathcal{W}_*} = \log\left(\frac{p(c_j|\mathcal{W}_*)}{p(c_j|\mathcal{W})}\right)$$

for every $c_j \in \mathcal{E}$.

Intuitively, "word sets paraphrase one another if they induce equivalent distributions over context words". When \mathcal{W} and \mathcal{W}_* paraphrase each other, we write $\mathcal{W} \approx_P \mathcal{W}_*$. From Definition 10, we observe that $\mathcal{W} \approx_P \mathcal{W}_*$ if and only if $\mathcal{W}_* \approx_P \mathcal{W}$. Also, we implicitly require both $p(\mathcal{W}_*)$ and $p(\mathcal{W})$ to be positive. This is exactly Assumption A3 in the original paper. We now provide an equivalent version of their Lemma 2 for the matrix M. Here, M_i^{\top} denotes the *i*-th row of M. The proof is provided in Appendix J.

Lemma 11. For any word sets $W, W_* \subseteq \mathcal{E}$ with the same cardinality, we have

$$\sum_{w_i \in \mathcal{W}_*} M_i = \sum_{w_i \in \mathcal{W}} M_i + \rho^{\mathcal{W}, \mathcal{W}_*} + \sigma^{\mathcal{W}} - \sigma^{\mathcal{W}_*} + \delta^{\mathcal{W}, \mathcal{W}}$$
$$= \sum_{w_i \in \mathcal{W}} M_i + \xi^{\mathcal{W}, \mathcal{W}_*} + \sigma^{\mathcal{W}} - \sigma^{\mathcal{W}_*},$$

where

$$\sigma_j^{\mathcal{W}} = \log\left(\frac{p(\mathcal{W}|c_j)}{\prod_{w_i \in \mathcal{W}} p(w_i|c_j)}\right),\$$
$$\sigma_j^{\mathcal{W}_*} = \log\left(\frac{p(\mathcal{W}_*|c_j)}{\prod_{w_i \in \mathcal{W}_*} p(w_i|c_j)}\right),\$$

 $\delta_j^{\mathcal{W},\mathcal{W}_*} = \log\left(\frac{p(\mathcal{W}_*)}{p(\mathcal{W})}\right)$, and $\xi_j^{\mathcal{W},\mathcal{W}_*} = \log\left(\frac{p(\mathcal{W}_*|c_j)}{p(\mathcal{W}|c_j)}\right)$.

Proposition 12, which is equivalent to Corollary 2.3 of Allen and Hospedales [2019], follows from multiplying both sides of the equations in Lemma 11 by $C^{\dagger} = (CC^{\top})^{-1}C$ (assuming C has full row rank) and setting $\mathcal{W} = \{w_b, w_{a^*}\}$ and $\mathcal{W}_* = \{w_{b^*}, w_a\}$.

Proposition 12. Given any $w_a, w_{a^*}, w_b, w_{b^*} \in \mathcal{E}$, we have

$$w_{b^*} = w_{a^*} - w_a + w_b + C^{\dagger}(\rho^{\mathcal{W},\mathcal{W}_*} + \sigma^{\mathcal{W}} - \sigma^{\mathcal{W}_*} + \delta^{\mathcal{W},\mathcal{W}_*})$$
$$= w_{a^*} - w_a + w_b + C^{\dagger}(\xi^{\mathcal{W},\mathcal{W}_*} + \sigma^{\mathcal{W}} - \sigma^{\mathcal{W}_*}),$$

where $W = \{w_b, w_{a^*}\}$ and $W_* = \{w_{b^*}, w_a\}$.

From Proposition 12, we see that when $\mathcal{W} \approx_P \mathcal{W}_*$, and $\sigma^{\mathcal{W}}$, $\sigma^{\mathcal{W}_*}$ and $\delta^{\mathcal{W},\mathcal{W}_*}$ are small, we have $w_{b^*} \approx w_{a^*} - w_a + w_b$. By definition, $\sigma^{\mathcal{W}} (\sigma^{\mathcal{W}_*})$ is small when all $w_i \in \mathcal{W} (w_i \in \mathcal{W}_*)$ are approximately conditionally independent given c_j , and $\delta^{\mathcal{W},\mathcal{W}_*}$ is small when $p(\mathcal{W}) \approx p(\mathcal{W}_*)$. Following the connection between analogies and word transformations described in Sections 6.3 and 6.4 of Allen and Hospedales [2019], we now have an approximately linear relationship for CBOW embeddings with some error terms mentioned above.

Alternatively, we can modify Definition 10 so that $\mathcal{W} \approx_P \mathcal{W}_*$ if and only if $\xi^{\mathcal{W},\mathcal{W}_*}$ (instead of $\rho^{\mathcal{W},\mathcal{W}_*}$) is element-wise small. Now, our error terms only depend on the approximate conditional independence of w_i 's given c_j .

Does this linear relationship also hold for context embeddings? In other words, if $w_r + w_s \approx w_t + w_u$, do we have $c_r + c_s \approx c_t + c_u$? Proposition 13, whose proof is provided in Appendix K, answers the question.

Proposition 13. Let $\mathcal{W} = \{r, s\}$ and $\mathcal{W}_* = \{t, u\}$. Assume $p(\mathcal{W}) \approx p(\mathcal{W}_*)$ and $w_i \in \mathcal{W}$ $(w_i \in \mathcal{W}_*)$ are approximately marginally independent. Also, assume that W has full row rank. If $w_r + w_s \approx w_t + w_u$, then $c_r + c_s \approx c_t + c_u$.

So far, we have argued that both the center and context embeddings of CBOW exhibit linear structures under some assumptions. We now extend this argument to MLM with self-attention, and show that the same conclusion holds under stronger assumptions.

G.2 Linear word analogies in attention-based embeddings

Similar to Section 4.2, we compute the matrix MLM with self-attention factorized and construct a paraphrasing argument to show linear structures in the learned embeddings.

What matrix does MLM with self-attention (approximately) factorize? To make calculations tractable, we exclude both residual connections and positional encodings. Let the masked sentence be (a_1, \dots, a_S) . As before, let $m \in [S]$ and $b \in [|V|]$ denote the masked position and masked word, respectively. This means $a_i \in [|V|]$ for every $i \neq m$ and $a_m = |V| + 1$. From Lemma 1, the loss for this instance is given by

$$-\sum_{j=1}^{S} \frac{\tau_{a_j}}{\sum_{j=1}^{S} \tau_{a_j}} w_b^{\top} c_{a_j} + \log\left(\sum_{k=1}^{|V|} \exp\left(\sum_{j=1}^{S} \frac{\tau_{a_j}}{\sum_{j=1}^{S} \tau_{a_j}} w_k^{\top} c_{a_j}\right)\right),$$
(1)

where $\tau_j = \exp\left(\frac{c_j^\top W^{KQ} c_{|V|+1}}{\sqrt{d_w}}\right)$. Proposition 14 approximates the matrix factorized by the attention objective, given all τ_j values for each $j \in [|V|+1]$. The proof is similar to that of Proposition 9, and therefore omitted.

Proposition 14. Consider the attention objective as in Equation (1). We have

$$w_{i}^{\top}c_{j} \approx \frac{|V|\sum_{(i,j)}\gamma_{j}^{i} - \left(\sum_{(1,j)}\gamma_{j}^{1} + \dots + \sum_{(|V|,j)}\gamma_{j}^{|V|}\right)}{S\left(\sum_{(1,j)}(\gamma_{j}^{1})^{2} + \dots + \sum_{(|V|,j)}(\gamma_{j}^{|V|})^{2}\right)},$$
(2)

where for a center-context pair (d, j) in the masked sentence (a_1, \cdots, a_S) , we define $\gamma_j^d = \tau_j / \sum_{s=1}^S \tau_{a_s}$.

In other words, MLM with self-attention approximately factorizes a $|V| \times |V|$ matrix whose (i, j)-th entry is given by Equation (2). It is important to note that unlike in CBOW, the token embedding for each word i is c_i (the *context* embedding), and not w_i (the *center* embedding). In the case where τ_j is approximately the same for every $j \in [|V| + 1]$, our problem approximately reduces to a vanilla CBOW. In particular, we always have $\gamma_j^d \approx 1/S$, whence Proposition 14 yields $w_i^{\top}c_j \approx \frac{p(w_i,c_j)}{p(c_j)} \cdot |V| - 1 \approx \log\left(\frac{p(w_i,c_j)}{p(c_j)}\right) + \log |V|$. Using Proposition 12, we argue that the resulting embeddings approximately form a linear relationship, up to some error terms.

The paraphrasing argument for MLM with self-attention. We first define

$$\tilde{c}_j := \frac{S\left(\sum_{(1,j)} (\gamma_j^1)^2 + \dots + \sum_{(|V|,j)} (\gamma_j^{|V|})^2\right)}{\sum_{(1,j)} \gamma_j^1 + \dots + \sum_{(|V|,j)} \gamma_j^{|V|}} c_j$$

for every $j \in [|V| + 1]$. This means

$$w_{i}^{\top} \tilde{c}_{j} \approx \frac{|V| \sum_{(i,j)} \gamma_{j}^{i}}{\sum_{(1,j)} \gamma_{j}^{1} + \dots + \sum_{(|V|,j)} \gamma_{j}^{|V|}} - 1$$
$$\approx \log \left(\frac{\sum_{(i,j)} \gamma_{j}^{i}}{\sum_{(1,j)} \gamma_{j}^{1} + \dots + \sum_{(|V|,j)} \gamma_{j}^{|V|}} \right) + \log |V|,$$

where we used the approximation $x \approx \log(1 + x)$. Previously, $p(w_i, c_j)$ represents a population quantity which is estimated by $\#(w_i, c_j)/D$, where D is a normalizing constant, and $p(c_j) = \sum_i p(w_i, c_j)$. We now define $\bar{p}(w_i, c_j)$, a population quantity which is estimated by $\sum_{(i,j)} \gamma_j^i/E$ for some normalizing constant E. We have

$$w_i^{\top} \tilde{c}_j \approx \log\left(\frac{\bar{p}(w_i, c_j)}{\bar{p}(c_j)}\right) + \log|V|,$$

where $\bar{p}(c_j) = \sum_i \bar{p}(w_i, c_j)$. Note that unlike p, \bar{p} is not symmetric, i.e., $\bar{p}(w_i, c_j) \neq \bar{p}(w_j, c_i)$. Having defined \bar{p} , we are ready to state Lemma 15, which is a version of Lemma 11 for the matrix N, where

$$N_{i,j} = \log\left(\frac{\bar{p}(w_i, c_j)}{\bar{p}(c_j)}\right) + \log|V|.$$

Here, N_i^{\top} denotes the *i*-th row of N. The proof is analogous to that of Lemma 11 and is thus omitted.

Lemma 15. For any word sets $\mathcal{W}, \mathcal{W}_* \subseteq \mathcal{E}$ with the same cardinality, we have

$$\sum_{w_i \in \mathcal{W}_*} N_i = \sum_{w_i \in \mathcal{W}} N_i + \bar{\rho}^{\mathcal{W}, \mathcal{W}_*} + \bar{\sigma}^{\mathcal{W}} - \bar{\sigma}^{\mathcal{W}_*} + \bar{\delta}^{\mathcal{W}, \mathcal{W}}$$
$$= \sum_{w_i \in \mathcal{W}} N_i + \bar{\xi}^{\mathcal{W}, \mathcal{W}_*} + \bar{\sigma}^{\mathcal{W}} - \bar{\sigma}^{\mathcal{W}_*},$$

where

$$\begin{split} \bar{\sigma}_{j}^{\mathcal{W}} &= \log\left(\frac{\bar{p}(\mathcal{W}|c_{j})}{\prod_{w_{i}\in\mathcal{W}}\bar{p}(w_{i}|c_{j})}\right),\\ \bar{\sigma}_{j}^{\mathcal{W}_{*}} &= \log\left(\frac{\bar{p}(\mathcal{W}_{*}|c_{j})}{\prod_{w_{i}\in\mathcal{W}_{*}}\bar{p}(w_{i}|c_{j})}\right),\\ \bar{\rho}_{j}^{\mathcal{W},\mathcal{W}_{*}} &= \log\left(\frac{\bar{p}(c_{j}|\mathcal{W}_{*})}{\bar{p}(c_{j}|\mathcal{W})}\right), \bar{\delta}_{j}^{\mathcal{W},\mathcal{W}_{*}} &= \log\left(\frac{\bar{p}(\mathcal{W}_{*})}{\bar{p}(\mathcal{W})}\right), \text{ and } \bar{\xi}_{j}^{\mathcal{W},\mathcal{W}_{*}} &= \log\left(\frac{\bar{p}(\mathcal{W}_{*}|c_{j})}{\bar{p}(\mathcal{W}|c_{j})}\right) \end{split}$$

Propositions 16 and 17 are the attention versions of Propositions 12 and 13. The proof of Proposition 16 follows from multiplying both sides of the equations in Lemma 15 by $\tilde{C}^{\dagger} = (\tilde{C}\tilde{C}^{\top})^{-1}C$ (assuming \tilde{C} has full row rank) and setting $\mathcal{W} = \{w_b, w_{a^*}\}$ and $\mathcal{W}_* = \{w_{b^*}, w_a\}$. The proof of Proposition 17 can be found in Appendix L.

Proposition 16. Given any $w_a, w_{a^*}, w_b, w_{b^*} \in \mathcal{E}$, we have

$$w_{b^*} = w_{a^*} - w_a + w_b + \tilde{C}^{\dagger}(\bar{\rho}^{\mathcal{W},\mathcal{W}_*} + \bar{\sigma}^{\mathcal{W}} - \sigma^{\mathcal{W}_*} + \bar{\delta}^{\mathcal{W},\mathcal{W}_*})$$

$$= w_{a^*} - w_a + w_b + \tilde{C}^{\dagger}(\bar{\xi}^{\mathcal{W},\mathcal{W}_*} + \bar{\sigma}^{\mathcal{W}} - \bar{\sigma}^{\mathcal{W}_*}),$$

where $W = \{w_b, w_{a^*}\}$ and $W_* = \{w_{b^*}, w_a\}$.

Proposition 17. Let $\mathcal{W} = \{r, s\}$ and $\mathcal{W}_* = \{t, u\}$. Assume $\bar{p}(\mathcal{W}) \approx \bar{p}(\mathcal{W}_*)$ and $w_i \in \mathcal{W}$ $(w_i \in \mathcal{W}_*)$ are approximately marginally independent. Also, assume that W has full row rank and $\bar{p}(w_i, c_j) \approx \bar{p}(w_j, c_i)$. If $w_r + w_s \approx w_t + w_u$, then $\tilde{c}_r + \tilde{c}_s \approx \tilde{c}_t + \tilde{c}_u$.

What do we learn from these results? One important takeaway is that the sufficient conditions to obtain linear relationships are stronger in the case of MLM with self-attention as compared to CBOW. Concretely, we need \bar{p} to be approximately symmetric. Even when this is satisfied, the linear relationships hold for the transformed embeddings \tilde{c}_i 's instead of the token embeddings c_i 's. Under an additional assumption that

$$\zeta_j := \frac{\sum_{(1,j)} (\gamma_j^1)^2 + \dots + \sum_{(|V|,j)} (\gamma_j^{|V|})^2}{\sum_{(1,j)} \gamma_j^1 + \dots + \sum_{(|V|,j)} \gamma_j^{|V|}}$$

is approximately the same for each j (e.g., when τ_j is approximately the same for every j), we approximately have linear relationships for the token embeddings c_i 's.

Remarks. It is easy to see that our result can technically be extended to incorporate positional encodings by considering each (word, position) pair as a unit. In particular, analogies are drawn between (word, position) units.

H Proof of Proposition 9

Proposition 9. Consider CBOW without negative sampling. Using the same notation as before, we have

$$w_i^{\top} c_j \approx \log\left(\frac{p(w_i, c_j)}{p(c_j)}\right) + \log|V|.$$

Proof. For simplicity, we assume that the window size is always 2m. Consider an instance with i as the center word and $j \in J$ as the context words. The loss for this instance can be approximated as

$$\begin{split} &-\frac{\sum_{j\in J} w_i^{\top} c_j}{2m} + \log\left(\sum_{k=1}^{|V|} \exp\left(\frac{\sum_{j\in J} w_k^{\top} c_j}{2m}\right)\right) \\ &\approx -\frac{\sum_{j\in J} w_i^{\top} c_j}{2m} + \log\left(\sum_{k=1}^{|V|} \left(1 + \frac{\sum_{j\in J} w_k^{\top} c_j}{2m} + \frac{(\sum_{j\in J} w_k^{\top} c_j)^2}{8m^2}\right)\right) \\ &= -\frac{\sum_{j\in J} w_i^{\top} c_j}{2m} + \log|V| + \log\left(1 + \frac{\sum_{k=1}^{|V|} \left(\sum_{j\in J} w_k^{\top} c_j\right)}{2m|V|} + \frac{\sum_{k=1}^{|V|} \left(\sum_{j\in J} w_k^{\top} c_j\right)^2}{8m^2|V|}\right) \\ &\approx -\frac{\sum_{j\in J} w_i^{\top} c_j}{2m} + \log|V| + \frac{\sum_{k=1}^{|V|} \left(\sum_{j\in J} w_k^{\top} c_j\right)}{2m|V|} + \frac{\sum_{k=1}^{|V|} \left(\sum_{j\in J} w_k^{\top} c_j\right)^2}{8m^2|V|} \\ &\leq -\frac{\sum_{j\in J} w_i^{\top} c_j}{2m} + \log|V| + \frac{\sum_{k=1}^{|V|} \left(\sum_{j\in J} w_k^{\top} c_j\right)}{2m|V|} + \frac{\sum_{k=1}^{|V|} \left(\sum_{j\in J} w_k^{\top} c_j\right)^2}{4m|V|}, \end{split}$$

where we used the Taylor expansions $\exp(x) \approx 1 + x + x^2/2$ and $\log(1 + x) \approx x$, as well as the Cauchy-Schwarz inequality. Ignoring the constant $\log |V|$ and multiplying by 2m|V|, the approximate loss can be written as

$$-|V|\sum_{j\in J} w_i^{\top} c_j + \sum_{k=1}^{|V|} \left(\sum_{j\in J} w_k^{\top} c_j\right) + \frac{1}{2} \sum_{k=1}^{|V|} \left(\sum_{j\in J} (w_k^{\top} c_j)^2\right).$$

Summing this over all instances and only extracting terms which depend on $w_i^{\top}c_j$, we have the following loss which we want to minimize:

$$\ell(i,j) = -|V| \cdot \#(w_i, c_j) w_i^{\top} c_j + \#(c_j) w_i^{\top} c_j + \frac{1}{2} \#(c_j) (w_i^{\top} c_j)^2.$$

Taking derivative with respect to $w_i^\top c_j$ and setting it to 0 yields

$$w_i^{\top} c_j = \left(\frac{\#(w_i, c_j)}{\#(c_j)}\right) \cdot |V| - 1 = \left(\frac{p(w_i, c_j)}{p(c_j)} \cdot |V|\right) - 1.$$

The approximation $x \approx \log(1+x)$ completes the proof.

I Corpus generation process

- 1. Consider four subjects (mathematics, statistics, sociology and history) and four adjectives (fun, boring, easy and difficult). Assign scores to each subject which represents the level of each adjective:
 - (a) mathematics: (4, 2, 4, 2).
 - (b) statistics: (6, 0, 5, 1).
 - (c) sociology: (1, 5, 2, 4).
 - (d) history: (0, 6, 0, 6).
- 2. Consider three types of sentence:
 - (a) Type 1: I like subj1 and subj2, where subj1 and subj2 are independently chosen from the list of subjects with probability (4/11, 5/11, 1/11, 1/11).
 - (b) Type 2: subj1 and subj2 is adj, where subj1 and subj2 are independently chosen from the list of subjects with uniform probability, and adj is chosen from the list of adjectives with probability proportional to the sum of the scores of subj1 and subj2.
 - (c) Type 3: subj is adj1 and adj2, where subj is chosen from the list of subjects with uniform probability, and adj1 and adj2 are independently chosen from the list of adjectives with probability proportional to the score of subj.
- 3. To generate each sentence, we first randomly choose the sentence type with uniform probability. We then form the sentence following the process above.

J Proof of Lemma 11

Lemma 11. For any word sets $W, W_* \subseteq \mathcal{E}$ with the same cardinality, we have

$$\sum_{w_i \in \mathcal{W}_*} M_i = \sum_{w_i \in \mathcal{W}} M_i + \rho^{\mathcal{W}, \mathcal{W}_*} + \sigma^{\mathcal{W}} - \sigma^{\mathcal{W}_*} + \delta^{\mathcal{W}, \mathcal{W}}$$
$$= \sum_{w_i \in \mathcal{W}} M_i + \xi^{\mathcal{W}, \mathcal{W}_*} + \sigma^{\mathcal{W}} - \sigma^{\mathcal{W}_*},$$

where
$$\sigma_j^{\mathcal{W}} = \log\left(\frac{p(\mathcal{W}|c_j)}{\prod_{w_i \in \mathcal{W}} p(w_i|c_j)}\right), \sigma_j^{\mathcal{W}_*} = \log\left(\frac{p(\mathcal{W}_*|c_j)}{\prod_{w_i \in \mathcal{W}_*} p(w_i|c_j)}\right), \delta_j^{\mathcal{W},\mathcal{W}_*} = \log\left(\frac{p(\mathcal{W}_*)}{p(\mathcal{W})}\right), and \xi_j^{\mathcal{W},\mathcal{W}_*} = \log\left(\frac{p(\mathcal{W}_*|c_j)}{p(\mathcal{W}|c_j)}\right).$$

$$\begin{aligned} \text{Proof. Observe that } p(c_j|\mathcal{W}_*) &= \frac{p(\mathcal{W}_*|c_j)p(c_j)}{p(\mathcal{W}_*)} \text{ and } p(c_j|\mathcal{W}) = \frac{p(\mathcal{W}|c_j)p(c_j)}{p(\mathcal{W})}, \text{ whence } \rho_j^{\mathcal{W},\mathcal{W}_*} = \\ \log\left(\frac{p(c_j|\mathcal{W}_*)}{p(c_j|\mathcal{W})}\right) &= \log\left(\frac{p(\mathcal{W}_*|c_j)}{p(\mathcal{W}|c_j)}\right) + \log\left(\frac{p(\mathcal{W}_*)}{p(\mathcal{W}_*)}\right). \text{ We have} \\ \sum_{w_i \in \mathcal{W}_*} M_i - \sum_{w_i \in \mathcal{W}} M_i &= \sum_{w_i \in \mathcal{W}_*} \log\left(\frac{p(w_i, c_j)}{p(c_j)}\right) - \sum_{w_i \in \mathcal{W}} \log\left(\frac{p(w_i, c_j)}{p(c_j)}\right) \\ &= \log\prod_{w_i \in \mathcal{W}_*} p(w_i|c_j) - \log\prod_{w_i \in \mathcal{W}} p(w_i|c_j) \\ &= \log\left(\frac{\prod_{w_i \in \mathcal{W}_*} p(w_i|c_j)}{\prod_{w_i \in \mathcal{W}} p(w_i|c_j)}\right) + \log\left(\frac{p(\mathcal{W}_*)}{p(\mathcal{W}_*)}\right) + \log\left(\frac{p(\mathcal{W})}{p(\mathcal{W})}\right) \\ &+ \log\left(\frac{p(\mathcal{W}_*|c_j)}{p(\mathcal{W}|c_j)}\right) + \log\left(\frac{p(\mathcal{W}|c_j)}{p(\mathcal{W}|c_j)}\right) \\ &= \log\left(\frac{p(\mathcal{W}_*|c_j)}{p(\mathcal{W}|c_j)}\right) + \log\left(\frac{p(\mathcal{W})}{p(\mathcal{W}_*)}\right) + \log\left(\frac{p(\mathcal{W}|c_j)}{\prod_{w_i \in \mathcal{W}} p(w_i|c_j)}\right) \\ &- \log\left(\frac{p(\mathcal{W}_*|c_j)}{\prod_{w_i \in \mathcal{W}_*} p(w_i|c_j)}\right) + \log\left(\frac{p(\mathcal{W}_*)}{p(\mathcal{W})}\right) \\ &= \rho_j^{\mathcal{W},\mathcal{W}_*} + \sigma_j^{\mathcal{W}} - \sigma_j^{\mathcal{W}_*} + \delta_j^{\mathcal{W},\mathcal{W}_*}.\end{aligned}$$

Also,

$$\rho_j^{\mathcal{W},\mathcal{W}_*} + \delta_j^{\mathcal{W},\mathcal{W}_*} = \log\left(\frac{p(\mathcal{W}_*|c_j)}{p(\mathcal{W}|c_j)}\right) + \log\left(\frac{p(\mathcal{W})}{p(\mathcal{W}_*)}\right) + \log\left(\frac{p(\mathcal{W}_*)}{p(\mathcal{W})}\right)$$
$$= \xi_j^{\mathcal{W},\mathcal{W}_*},$$

which completes the proof.

K Proof of Proposition 13

Proposition 13. Let $\mathcal{W} = \{r, s\}$ and $\mathcal{W}_* = \{t, u\}$. Assume $p(\mathcal{W}) \approx p(\mathcal{W}_*)$ and $w_i \in \mathcal{W}$ $(w_i \in \mathcal{W}_*)$ are approximately marginally independent. Also, assume that W has full row rank. If $w_r + w_s \approx w_t + w_u$, then $c_r + c_s \approx c_t + c_u$.

Proof. For any $c_v \in \mathcal{E}$, we have $(w_r + w_s)^{\top} c_v \approx (w_t + w_u)^{\top} c_v$. From Proposition 3, this expression can be simplified as $\log p(w_r, c_v) + \log p(w_s, c_v) \approx \log p(w_t, c_v) + \log p(w_u, c_v)$. This implies $\log p(w_v, c_r) + \log p(w_v, c_s) \approx \log p(w_v, c_t) + \log p(w_v, c_u)$. Observe that

$$w_v^{\scriptscriptstyle +}(c_r + c_s - c_t - c_u) = (\log p(w_v, c_r) + \log p(w_v, c_s) - \log p(w_v, c_t) - \log p(w_v, c_u)) + \log \left(\frac{p(c_t)p(c_u)}{p(c_r)p(c_s)}\right)$$
$$\approx 0 + \log \left(\frac{p(\mathcal{W}_*)}{p(\mathcal{W})}\right)$$
$$\approx 0.$$

Since this holds for every v and W has full row rank, we conclude that $c_r + c_s \approx c_t + c_u$, completing the proof.

L Proof of Proposition 16

Proposition 16. Let $\mathcal{W} = \{r, s\}$ and $\mathcal{W}_* = \{t, u\}$. Assume $\bar{p}(\mathcal{W}) \approx \bar{p}(\mathcal{W}_*)$ and $w_i \in \mathcal{W}$ $(w_i \in \mathcal{W}_*)$ are approximately marginally independent. Also, assume that W has full row rank and $\bar{p}(w_i, c_j) \approx \bar{p}(w_j, c_i)$. If $w_r + w_s \approx w_t + w_u$, then $\tilde{c}_r + \tilde{c}_s \approx \tilde{c}_t + \tilde{c}_u$.

Proof. For any $\tilde{c}_v \in \mathcal{E}$, we have $(w_r + w_s)^{\top} \tilde{c}_v = (w_t + w_u)^{\top} \tilde{c}_v$. From Appendix G.2, this expression can be simplified as $\log \bar{p}(w_r, c_v) + \log \bar{p}(w_s, c_v) \approx \log \bar{p}(w_t, c_v) + \log \bar{p}(w_u, c_v)$. By the assumption that $\bar{p}(w_i, c_j) \approx \bar{p}(w_j, c_i)$, this implies $\log \bar{p}(w_v, c_r) + \log \bar{p}(w_v, c_s) \approx \log \bar{p}(w_v, c_t) + \log \bar{p}(w_v, c_u)$. Observe that

$$w_v^{\top}(\tilde{c}_r + \tilde{c}_s - \tilde{c}_t - \tilde{c}_u)$$

$$= (\log \bar{p}(w_v, c_r) + \log \bar{p}(w_v, c_s) - \log \bar{p}(w_v, c_t) - \log \bar{p}(w_v, c_u)) + \log \left(\frac{\bar{p}(c_t)\bar{p}(c_u)}{\bar{p}(c_r)\bar{p}(c_s)}\right)$$

$$\approx 0 + \log \left(\frac{\bar{p}(\mathcal{W}_*)}{\bar{p}(\mathcal{W})}\right)$$

$$\approx 0.$$

Since this holds for every v and W has full row rank, we conclude that $\tilde{c}_r + \tilde{c}_s \approx \tilde{c}_t + \tilde{c}_u$, completing the proof.