On a Benefit of Masked Language Model Pretraining: Robustness to Simplicity Bias

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Abstract

Despite the success of pretrained masked language models (MLM), why MLM pretraining is useful is still a question not fully answered. In this work we theoretically and empirically show that MLM pretraining makes models robust to lexicon-level spurious features, partly answering the question. Our explanation is that MLM pretraining may alleviate problems brought by simplicity bias (Shah et al., 2020), which refers to the phenomenon that a deep model tends to rely excessively on simple features. In NLP tasks, those simple features could be token-level features whose spurious association with the label can be learned easily. We show that MLM pretraining makes learning from the context easier. Thus, pretrained models are less likely to rely excessively on a single token. We also explore the theoretical explanations of MLM's efficacy in causal settings. Compared with Wei et al. (2021), we achieve similar results with milder assumptions. Finally, we close the gap between our theories and real-world practices by conducting experiments on real-world tasks.

1 Introduction

The question "*why is masked language model (MLM) pretraining (Devlin et al., 2019; Liu et al., 2019) useful?*" has not been totally answered. In this work, as an initial step toward the answer, we show and explain that MLM pretraining makes the model robust to lexicon-level features that are spuriously associated with the target label. It gives the model a better generalization capability under distribution shift.

Previous studies have empirically shown the robustness of MLM pretrained models. Hao et al. (2019) show that MLM pretraining leads to wider optima and better generalization capability. Hendrycks et al. (2020) and Tu et al. (2020) show that pretrained models are more robust to out-of-distribution data and spurious features. However, it remains unanswered why pretrained models are more robust.

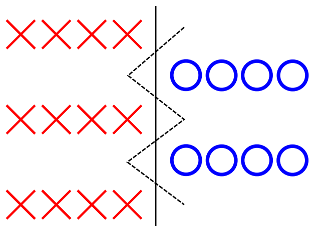


Figure 1: The pitfall of simplicity bias: The solid line is a simple (linear) decision boundary that utilizes only one dimension, while the dashed line is a more complex decision boundary that utilizes two dimensions and maximizes the margin.

We conjecture that models trained from scratch suffer from the pitfall of simplicity bias (Shah et al., 2020) (Figure 1). Shah et al. (2020) and Kalimeris et al. (2019) showed that deep networks tend to converge to a simple decision boundary that involves only a few features. The networks may not utilize all the features and thus may not maximize the margin, which results in worse robustness. A consequence of this could be that a model may excessively rely on a feature that has spurious association with the label and ignore the other features that are more robust. In the studies of Shah et al. (2020) and Kalimeris et al. (2019), they investigated networks with continuous input. Lovering et al. (2021) discovered similar results on synthetic NLP tasks, where the inputs are discrete. We will further explore this discrete setting in this work.

We start the exploration with the following assumptions: Let the sentence, label pair be X, Y.

Assumption 1. *We assume that from X, we can extract two features X_1 and X_2.*

Assumption 2. *X_1 is a spurious feature that has strong association with Y. Specifically, it means that, solely relying on X_1, one can predict with high accuracy over the data distribution, but cannot be 100% correctly.*

Assumption 3. *X_2 is a robust feature based on which Y can be predicted with 100% accuracy. Namely, there exists a deterministic mapping $f_{X_2 \to Y}$ that maps X_2 to Y.*

The assumptions above are realistic in some NLP tasks. In NLP tasks, the input X is a sequence of tokens. Some tasks satisfy Assumption 1: X can be decomposed into X_1 and X_2, where X_1 is the presence of certain tokens, and X_2 is the context of the token. Thus, X_2 has a much higher dimensionality than X_1. As shown by the analysis of Gardner et al. (2021), there are indeed datasets where Assumption 2 is true. However, if Assumption 3 is true, we would desire the model to rely on X_2, which contains the semantics of the input X.

With these assumptions, in Section 2 we empirically demonstrate that spurious features in discrete inputs can cause problems as in the continuous cases (Shah et al., 2020; Kalimeris et al., 2019). We show that, possibly due to the simplicity bias, a deep model is likely to excessively rely on X_1 and to rely on X_2 less. In Section 3.1 and Section 3.2 we provide a theoretical explanation of how MLM pretraining makes a model robust to spurious features. Let Π_1 be the conditional probability $P(X_1|X_2)$. We show (1) the relation between the mutual information $I(\Pi_1; Y) \geq I(X_1; Y)$ and that (2) the convergence rate of learning from Π_1 is of the same order as learning from X_1. That is, when the MLM model can perfectly model the probability $P(X_1|X_2)$ and thus generate perfect Π_1, learning from Π_1 is as easy as learning from X_1. As a result, the model will be more likely to rely on Π_1. Since Π_1 is estimated based on X_2, higher reliance on Π_1 also implies higher reliance on the robust feature X_2. This avoids the pitfall of simplicity bias that the model relies excessively on X_1. To relax Assumption 3, we make one step further by considering causal settings in Section 3.3.

The above results partly explain why MLM pretrining is useful for NLP. Denote a sequence of tokens as $X = \langle X_1, X_2, \cdots, X_L \rangle$. During the MLM pretraining process, each token is masked randomly at a certain probability, and the training objective is to predict the masked tokens with the maximum likelihood loss. As a result, the model is capable of estimating the conditional probability $P(X_i|X \setminus X_i)$ for all $i = 1, 2, \cdots, L$. Even though which of the tokens is spurious is unknown, as long as the spurious token has a non-zero probability to be masked during pretraining, MLM can estimate its distribution conditioned on the context and thus can reduce the reliance on it.

Finally, we close the gap between our theories and reality. One major gap is that, in reality, we do not use the conditional probability for downstream tasks. Instead, we feed the input X without masking any token and fine-tune the model along with a shallow layer over its output. Regardless of that, we hypothesize that the robustness brought by MLM pretraining still exists. To prove that, in Section 4 we use the toy example and verify the effect of MLM pretraining when using the common practice for fine-tuning. In Section 5, we validate our theories with two real-world NLP tasks.

To sum up, our study leads to new research directions. Firstly, we provide a new explanation of MLM pretraing's efficacy. Unlike the previous purely theoretical studies (Saunshi et al., 2021; Wei et al., 2021), our assumptions are milder and more realistic. Secondly, we study NLP robustness from the perspective of self-supervised model. Since self-supervised trained embeddings have been widely used since Word2vec (Mikolov et al., 2013), it is indispensable to the generalization to unseen data. We reveal the mechanism that leads to its robustness, which may enable us to further reinforce it in the future.

2 A Toy Example

To show that spurious association can cause difficulty of convergence, we construct a toy example with variables X_1, X_2, Y that satisfy the assumptions. We make X_1 depends only on X_2, so it is not a causal feature of Y. Let the dimension of the random variables X_1 and X_2 be 2 and d_2 respectively. Their value $x_1 \in \mathcal{X}_1 = \{e_1, e_2\}$ and $x_2 \in \mathcal{X}_2 = \{e_1, \cdots, e_{d_2}\}$, where e_i is the one-hot vector whose ith element is 1. We control the strength of the association between X_1 and Y with $\nu < 0.5$, making $X_1 = Y$ with probability $1 - \nu$. Specifically, denote with $\dot{X}_2$ the middle $2\nu d_2$ dimensions of X_2, i.e. the $\lfloor d_2/2 - \nu d_2 \rfloor$th to the $\lfloor d_2/2 + \nu d_2 \rfloor$th elements in X_2. We consider the following random process:

$$X_2 = e_i, i \sim \text{Uniform}(1, d_2)$$
$$Y = \begin{cases} -1 & \text{if } X_2 = e_i \text{ for some } i < d_2/2 \\ +1 & \text{otherwise} \end{cases} \quad (1)$$
$$X_1 = \begin{cases} e_i, i \sim \text{Uniform}(1, 2) & \text{If } \dot{x}_2 \neq 0 \\ f(X_2) & \text{Otherwise} \end{cases},$$

		1 layer	2 layers		3 layers	
d_2	ν	w/o	w/o pre	w/ pre	w/o pre	w/ pre
50	0.04	3680 (189.5)	691 (55.8)	614 (169.1)	302 (47.2)	249 (53.7)
	0.10	2664 (121.2)	530 (30.6)	441 (134.9)	242 (27.6)	180 (37.5)
	0.25	1420 (96.0)	352 (23.8)	300 (62.0)	179 (13.8)	148 (28.7)
	0.50	306 (79.8)	141 (40.7)	118 (33.4)	106 (23.1)	89 (24.0)
100	0.04	5466 (170.1)	945 (57.2)	689 (225.3)	431 (51.1)	275 (72.1)
	0.10	3789 (99.2)	677 (32.2)	478 (142.9)	317 (30.3)	208 (44.3)
	0.25	1952 (64.9)	428 (13.1)	330 (85.0)	214 (16.2)	169 (32.5)
	0.50	330 (78.0)	156 (34.0)	133 (41.2)	128 (28.2)	112 (36.1)
500	0.04	11127 (265.9)	1953 (112.5)	857 (442.6)	792 (69.8)	431 (88.4)
	0.10	7912 (169.2)	1279 (67.5)	657 (234.9)	550 (46.7)	402 (97.0)
	0.25	4321 (152.3)	772 (35.5)	501 (133.5)	399 (42.3)	391 (66.0)
	0.50	576 (150.0)	392 (70.2)	407 (81.1)	367 (69.1)	386 (80.0)

Table 1: The number of iterations a model w/ or w/o pretraining requires to converge. The number is the average of 25 runs with different random seeds, and the number in parentheses is the standard deviation.

where $f(X_2) = e_1$ if $X_2 = e_i$ for some $i < d_2/2$, and $f(X_2) = e_2$ otherwise [1]. In this way, predicting Y solely based on the spurious feature X_1 can achieve accuracy $1 - \nu$.

We conduct experiments to inspect the effect of the strength of spurious association between X_1 and Y. We train linear networks by drawing batches of i.i.d. $([X_1; X_2], Y)$ pairs from the random process defined in Equation 1. We use Adam optimization with learning rate 0.001 and the cross-entropy loss. In addition to single-layer linear networks, we also try over-parameterized 2-layer and 3-layer linear networks. The hidden size is [10, 32]. Since it is a linearly separable problem, we can check whether the learned weight can lead to 100% accuracy in the defined distribution. We check it every 25 iterations. We say a model has converged if it is 100% accurate for 5 consecutive checks. We report the number of the iterations required before it converges for different ν and d_2.

Even though it is a linear-separable convex optimization problem, our results in Table 1 show that the strength of the spurious association can impact the number of iterations required to converge. We observe that when $\nu < 0.5$, the models tend to be trapped by the spurious feature, sticking at accuracy $1-\nu$ for iterations. When the spurious relation between X_1 and Y is stronger, i.e. ν is smaller, the number of iterations required to converge is larger. In addition, the number of iterations is also larger when the d_2 is larger. An intuitive explanation is that the learning signal from X_2 is more sparse when d_2 is larger.

3 A Theoretical Explanation of the Efficacy of MLM Pretraining

3.1 $P(X_1|X_2)$ is More Informative Than X_2

The toy example above motivates us to consider the information contained in $P(X_1|X_2)$. In the toy example, when predicting $P(Y = 0|X)$, if we simply output $P(X_1 = e_1|X_2)$, then the accuracy of our prediction of Y will be as high as predicting Y solely based on X_1. It motivates us to inspect the reliability of the estimated $P(X_1|X_2)$ as a feature for the prediction of Y compared to X_1. Let Π_1 be a $|\mathcal{X}_1|$-dimensional random variable whose value is $P(X_1|X_2)$ [2]. We can prove that when $P(X_1|X_2)$ is estimated perfectly, Π_1 is at least as informative as X_1.

Lemma 1. *When X_1, X_2 are discrete, if Π_1 perfect, namely the value of Π_1 is exactly $P(\cdot|X_2)$, then the mutual information $I(X_1; \Pi_1) = I(X_1; X_2)$. (Proof: Appendix A.1)*

Compared to previous works (Hjelm et al., 2019; Belghazi et al., 2018; Oord et al., 2018; Kong et al., 2020) that show some self-supervised training objectives are lower bounds of the mutual information $I(X_1; X_2)$, we directly show that the output of the MLM, Π, maximizes the mutual information, since $I(X_1; f(X_2)) \leq I(X_1; X_2)$ for any f. Moreover,

[1] $\text{Uniform}(a, b)$ is the uniform distribution over $\{n\}_{n=a}^{b}$.

[2] We will omit the subscript of Π_1 when there is no ambiguity.

instead of explaining the efficacy of pretraining with the infomax principle (Linsker, 1988; Bell and Sejnowski, 1995), our theories below provide a different perspective.

Theorem 1. *If* Π *is perfect,*

$$I(\Pi; Y) \geq I(X_1; Y) \tag{2}$$

Proof. Since Π is perfect, by Lemma 1, we have

$$I(X_1; X_2) = I(X_1; \Pi). \tag{3}$$

By data processing inequality, Equation 3 implies $I(X_1; X_2|\Pi) = 0$. By Assumption 3, a deterministic mapping $f_{X_2 \to Y}$ from X_2 to Y exists. Applying data processing inequality again, we have

$$\begin{aligned} I(X_1, X_2|\Pi) &\geq I(X_1, f_{X_2 \to Y}(X_2)|\Pi) \\ &= I(X_1, Y|\Pi) \geq 0, \end{aligned} \tag{4}$$

which implies $I(Y, X_1|\Pi) = 0$. Accordingly,

$$H(Y|\Pi) = H(Y|X_1, \Pi) \leq H(Y|X_1) \tag{5}$$

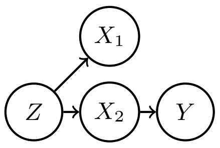
□

Theorem 1 shows that Π is a more informative feature than X_1. However, a model does not necessarily rely more on a more informative feature. We will discuss more in the next section.

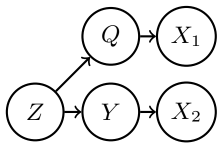
3.2 Learning from Π is Easy

It is important that learning from Π is easy. Because of simplicity bias, a neural network model is likely to rely on the easy-to-learn features (Shah et al., 2020; Kalimeris et al., 2019). We conjecture that a model excessively relies on the spurious feature X_1 when learning from X_1 is easier than learning from the robust feature X_2. If learning from Π is easy, then the model will rely on Π more and thus will rely on X_1 less. However, features with higher mutual information to Y are not necessarily easy to learn. For instance, although X_2 is more informative, models tend to rely on X_1 instead of X_2 at the beginning of the training process. To show that MLM can mitigate the issue brought by simplicity bias, we need to show learning from Π is easy.

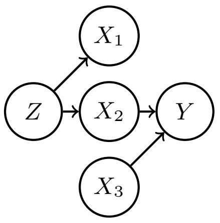
Therefore, we have the following theorem that implies learning from Π is at least as easy as learning from X_1:



(a) Causal setting



(b) Anticausal setting



(c) A case where $I(\Pi_3; Y) \geq I(\Pi_1; Y)$ is possible.

Figure 2: The causal settings of the (X, Y) pairs.

Theorem 2. *Let* $\tilde{h}_{X_1}^{(D_n)} : \mathcal{X}_1 \to \mathcal{Y}$ *be the classifier trained with MLE loss using* n *data pairs* $(x_1^{(1)}, y^{(1)}), (x_1^{(2)}, y^{(2)}), \cdots (x_1^{(n)}, y^{(n)})$, *and the converged classifier be* $\tilde{h}_{X_1}^*$. *There exists a learning algorithm, which generates* $\tilde{h}_{\Pi}^{(D_n)} : \Pi \to \mathcal{Y}$ *using* $(\Pi_1, y^{(1)})$, $(\pi^{(2)}, y^{(2)})$, $\cdots$, $(\pi^{(n)}, y^{(n)})$, *such that the following three properties are satisfied: (1)*

$$\mathbb{E}\left[D_{KL}\left[\tilde{h}_{\Pi}^{(D_n)} \,\middle\|\, \tilde{h}_{\Pi}^*\right]\right] = O\left(\frac{1}{n}\right), \tag{6}$$

which is asymptotically at the same rate as $\mathbb{E}\left[D_{KL}\left[\tilde{h}_{X_1}^{(D_n)} \,\middle\|\, \tilde{h}_{X_1}^*\right]\right]$. *(2) Over the distribution of* (X, Y), *the expected loss of the converged classifier* $\tilde{h}_{\Pi}^*$ *is not greater than the expected loss of* $\tilde{h}_{X_1}^*$. *(3)* $\tilde{h}_{\Pi}^*$ *is a linear model, whose input is* Π. *(Proof: Appendix A.2)*

The remaining question is whether deep learning models used in common practices can perform at least as well as the algorithm in Theorem 2. Indeed, without any knowledge of deep learning models, it is impossible to theoretically prove that a model will necessarily rely on Π instead of X_1. Therefore, in Section 4 and Section 5 we will empirically validate that our theorems are applicable in the real world scenarios.

3.3 Extending with Causal Models

We make a step further by relaxing Assumption 3. We do so by treating X_1 as a confounder, and then we can see how MLM pre-training is helpful in the causal and anticausal settings as in Kaushik et al. (2021).

	Ours	Wei et al. (2021)
structural assumption	X, Y follow Figure 2b.	X, Y follow an HMM.
linear independence assum.	$\{P(X_1\|y)\|y \in \mathcal{Y}\}$	$\{P(X_0\|H_0 = h)\|h \in \mathcal{H}\}$
implication	$I(P(X_1\|X_2); Y) = I(X_2; Y)$	$I(P(H_0\|X); Y) = I(X; Y)$

Table 2: Comparison between Theorem 4 in this work and Theorem 3.3 in Wei et al. (2021).

Theorem 3. *Even if Assumption 3 is not true, Theorem 1 still holds if X_1, X_2, Y follow the causal setting in Figure 2a.*

Proof. By the structure of X_1, X_2, Y, inequality 4 holds even if the deterministic mapping $f_{X_2 \to Y}$ does not exist. $\square$

Theorem 4. *Assume that the set of vectors $\{P(X_1|Y = y)|y \in \mathcal{Y}\}$ is linear independent, and if X_1, X_2, Y follow the anticausal setting in Figure 2b, then $I(\Pi; Y) \geq I(X_2; Y)$.*

Proof. The assumption is a special case of the one in (Lee et al., 2020), so similar techniques can be used: According to the structure of X_1, X_2, Y, we have

$$P(X_1|X_2) = \sum_y P(X_1|y)P(y|X_2). \quad (7)$$

Therefore, if $\{P(X_1|Y = y)|y \in \mathcal{Y}\}$ is linearly independent, $P(y|X_2)$ can be recovered from $\Pi = P(X_1|X_2)$. $\square$

Note that this theorem is very similar to Theorem 3.3 in Wei et al. (2021). However, the assumptions required in ours are weaker and more realistic, and the implication is very similar (Table 2): **(1) Structure assumption:** Wei et al. (2021) assumed that X is generated from a HMM process with hidden variables $H_0, H_1, \cdots$, which is stronger assumption than our assumption that X_1, X_2 follow the anticausal setting. **(2) Independence assumption:** Wei et al. (2021) assumed that the vectors in $\{P(X_0|H_0 = h)|h \in \mathcal{H}\}$ need to be linearly independent. In comparison, we require only the independence in $\{P(X_1|Y = y)|y \in \mathcal{Y}\}$. Our assumption is more realistic because the number of hidden states $|\mathcal{H}|$ must be very large if X is generated from the HMM model, and $|\mathcal{Y}|$ tends to be much smaller than $|\mathcal{H}|$. For example, in binary classification cases, our assumption holds as long as $P(X_1)$ is not independent of $P(Y)$. **(3) Implication:** If we further assume that $I(X_2; Y) = I(X; Y)$, then we reach a similar conclusion that $P(Y|X)$ can be recovered from $\Pi = P(X_1|X_2)$ by applying a linear function.

3.4 Limitations of Our Theorems

Our theories do not ensure that Π_1 is the most informative feature to learn from. Consider tokens in a sentence $X = \langle X_1, X_2, \cdots, X_L \rangle$ and let Π_i be the conditional probability $P(X_i|X \setminus X_i)$. A token with spurious association with the label can locate arbitrary position in the sentence, and its location is unknown during pretraining. That is, the pretrained model is able to generate Π_i for all i. Without loss of generality, assume X_1 is the spurious token. *It is possible that there exists some i such that $I(\Pi_1; Y) < I(\Pi_i; Y)$, and that Π_i is predicted relying on X_1.* Concretely, here is an example for the causal setting with three features: X_3 is independent of X_1 and X_2 given Y (Figure 2c). Using the results in Theorem 4, there is a linear mapping that can recover $P(Y|X_1, X_2)$ from Π_3. Therefore, it is possible that $I(\Pi_3; Y) > I(\Pi_1; Y)$ if $I(X_1, X_2; Y) > I(\Pi_1; Y)$ depending on the distribution of the data. We leave the study of $I(\Pi_i; Y)$ for future work.

Another limitation is that, in practice, NLP practitioners do not use the conditional probability predicted by the pretrained model. Instead, people stack a simple layer over the pretrained model, and fine-tune the whole model on downstream tasks. Regardless of this, we conjecture that the representation encoded by an MLM pretrained model still contains the information of $\{\Pi_i\}_{i=1}^n$ and thus is robust to spurious lexicon-level feature.

4 Toy Example with a Pretrained Model

As the first step to close the gap between our theories and the real world, we repeat the toy experiments with pretraining. Before fitting the model with Y, we first pretrain the first layer to predict X_1 based on masked X. What we want to show is that, after pretraining, the representation encoded by the layer will have the equivalent role of Π even when the input is not masked.

Specifically, the experimental design is as follows: We use the two-layer and three-layer MLP architectures same as in Section 2. When pretraining, we mask X_1 in X by using $X' = [0, 0; X_2]$ as inputs. Let the output from the first linear layer as $Z = WX'$. The loss function is the cross-entropy between X_1 and the softmax over $[z_1, z_2]$. After pretraining, we fine-tune the pretrained model with $([X_1; X_2], Y)$ pairs, and report the average number of iterations required to converge for 25 different random seeds.

We want to eliminate the possibility that the faster convergence of the pretrained model is because of larger initial weights over X_1. Therefore, after pretraining, we manually create a path from X_1 to Z. We do so by initializing the weights of the third and fourth row of W with $[k, -k, 0, \cdots, 0]$ and $[-k, k, \cdots, 0, 0]$ respectively, where k is the average of the absolute value of the weights in the pretrained part, i.e. the weights of the first two rows in W. In this way, the information from X_1 has the same scale as the pretrained representation $[Z_1, Z_2]$, and thus it can compete with $[Z_1, Z_2]$ fairly.

Table 1 shows that pretraining can always reduce the number of iterations required to converge when $\nu < 0.50$. The effect is more significant when d_2 is larger. It could be because of the higher sparsity of the learning signal from X_2 when d_2 is larger.

We further inspect how the importance over the inputs changes in the process of training. The importance can be inferred from the product of the linear layers. We observe that if the model is not pretrained, the weights over X_1 grow faster than the weights over X_2 at the beginning (the first row Figure 3). The model cannot converge to 100% accuracy until weights on $\dot{X}_2$, the middle $\lceil \nu \times d_2 \rceil$ dimensions of X_2, become greater than the weights on X_1. In addition, after the model converges, weights over X_1 is still greater than weights over X_2. On the other hand, if the model is pretrained, weights over X_1 stop growing after a few steps (the second row in Figure 3). The above observations are aligned with our conjecture that the pretrained representation mitigates the robustness issue brought simplicity bias.

5 Experiments

We experiment on real world NLP tasks to verify the relation between the capability of modeling the distribution of spurious features Π_1 and robustness. We facilitate datasets with known spurious features.

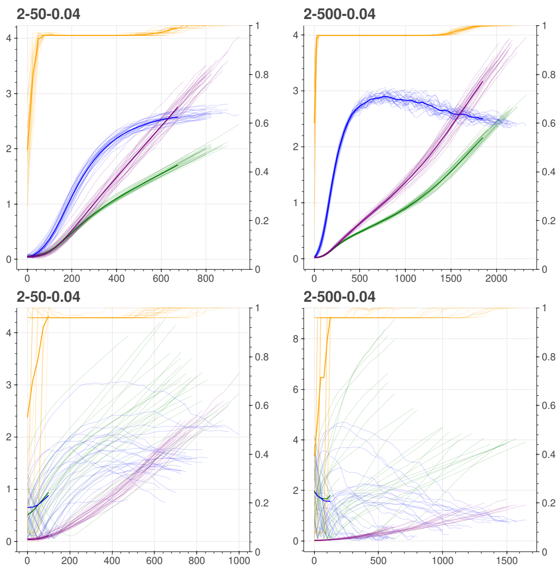


Figure 3: The average weights over the features during training a two-layer model. The upper and the lower rows are the curves of model without and with pretraining respectively. From left to right, $(d_2, \nu) = (50, 0.04), (500, 0.04)$. Blue, green, purple curves represent the average weights over features in X_1, X_2, and $\dot{X}_2$ (the middle part of X_2) respectively. The orange curve represents the accuracy.

We first pretrain models on the training dataset with different masking policies. One of them does not mask the spurious tokens, leading to the reduced capability of modeling Π_1. Afterward, we fine-tune the model using the target label. We show that the models are less robust on downstream tasks if spurious tokens are not masked during pretraining, which validates our theories.

5.1 Dowstream Tasks

Hate Speech Detection Previous study has shown that hate speech detection datasets tend to have lexical bias (Dixon et al., 2018). That is, models rely excessively on the presence or the absence of certain words when predicting the label. Here we follow the formulation of lexical bias in hate speech detection proposed by Zhou et al. (2021). We focus on the effect of non-offensive minority identity (NOI) mentions, such as “woman”, “gay”, “black”. Those mentions are often highly associated with hateful instances. However, it is more desirable that a model does not rely on those mentions. Therefore, we can see the presence of NOI as a spurious feature.

Name Entity Recognition (NER) Lin et al. (2020) has shown that name entity recognition

(NER) models perform worse when the name entities are not seen in the training data. In this case, we can see the content of the name entities as a spurious feature. Models may learn to memorize the name entities when fitting the training data, while we may desire the model to recognize name entities according to the context.

5.1.1 Datasets

Hate Speech Detection We use a portion of the dataset proposed by Founta et al. (2018). In their original dataset, only a small number of hateful instances contain NOI. Our preliminary experiments show that the model without pretraining does not suffer much from the bias of NOI when training with the full data. Therefore, we create a dataset, whose positive (hateful) instances are all the positive samples in the original dataset that contain NOI. As for negative instances, we sample them randomly from the original training set. We control the number of negative instances so the ratio of positive and negative instances is the same as the original dataset. We create both the training and the validation splits in this way, and use the original full testing set for evaluation. We also evaluate the models on a NOI subset where all the instances contain NOI.

NER We use the standard NER dataset Conll-2003 (Tjong Kim Sang and De Meulder, 2003). To create a testing set with name entities unseen in the training set, we replace the name entities in the original validation and testing splits with the entities from WNUT-17 (Derczynski et al., 2017). Specifically, we replace the `LOC`, `ORG`, `PER` entities with the corresponding type of entities in WNUT-17, while the `MISC` entities remain untouched.

5.2 Masking Policies

For each sentence with n_s spurious tokens, we experiment with different masking policies: **(1) scratch**: We do not pretrain the model before fine-tuning. **(2) vanilla**: During pretraining, we mask each token with 15% probability, which is same as the original implementation in (Devlin et al., 2019). **(3) unmask random**: This is similar to vanilla MLM, but we uniformly randomly select n_s tokens from the whole sentence and unmask them if they have been masked. **(4) unmask spurious**: This is similar to vanilla MLM, but we unmask all the spurious tokens. **(5) remove spurious**: We replace spurious tokens with a special "[unk]" token, and we unmask them. Note that this setting can be seen as an oracle setting, since in most applications the spurious features are unknown.

We will inspect the effect of masking spurious tokens by comparing setting (3), (4), (5). Note that these three setting have the same expected number of masked tokens. Therefore, it rules out the possibility that their downstream performance differs because of the number of masked tokens.

5.3 Implementation Details

For both of the tasks and all the MLM settings, including the *scratch setting*, we tokenize the input with the bert-base-uncased tokenizer. We use the bert-base-uncased architecture and also the pretrained embedding layer, which is frozen through the pretraining process. We repeat each experiment 5 times. We include more details in Appendix A.4.

5.4 Result and Discussion

Results in Table 3 validate our theorems. For both of the tasks, *unmask random* performs better than *unmask spurious* under distribution shift. Specifically, *unmask random* has higher F1 on the unseen set of the NER task, and *unmask random* has a lower false positive rate (FPR) on the NOI set. Also, *unmask random* performs similarly to *vanilla*. This implies that modeling the condition distribution of spurious tokens in the original random masking pretraining can reduce models' reliance on them. Note that *unmask random* and *unmask spurious* have similar in-distribution performance, so the performance difference is not due to better in-distribution generalization suggested by Miller et al. (2021).

We also compare *unmask random* with the oracle setting *remove spurious*. We notice that even though *remove spurious* performs as well as *random*, *remove spurious* hurts the performance in the seen set. It indicates that modeling the conditional distribution of spurious tokens has effects beyond simply removing them from the model. On the other hand, *remove spurious* performs better in the hate speech detection task. A possible explanation is that NOI mentions contain little useful information for the task.

6 Related Work

Recently, there are efforts attempting to explain the effectiveness of massive language modeling pretraining. Theoretically, Saunshi et al. (2021)

Mask Policy	NER		Hate Speech Detection			
	Origin	Unseen	All (12893)		NOI (602)	
	F1 ↑	F1 ↑	Accuracy ↑	F1 ↑	Accuracy ↑	FPR ↓
scratch	61.5 0.5	38.7 0.6	83.9 1.6	80.3 1.4	74.8 1.5	46.3 7.2
vanilla	74.2 0.4	56.5 1.3	83.1 0.8	78.5 0.8	75.8 0.5	25.1 1.8
unmask random	72.7 0.6	56.5 0.8	83.3 1.1	78.9 1.1	75.8 0.9	25.7 2.3
unmask spurious	72.9 0.5	53.2 0.8	84.1 0.7	79.8 0.6	73.7 1.0	32.5 2.1
remove spurious	69.8 0.5	56.7 0.8	82.4 1.0	77.8 1.0	77.3 0.6	21.7 2.0

Table 3: The performance on downstream tasks. For the hate speech detection task, we also report false positive detection (FPR) on the NOI subset, which is a set of instances containing non-offensive minority identity mentions, e.g. "women", "black". The results are the average of 5 runs, and the smaller number is the standard deviation.

explore why auto-regressive language models help solve downstream tasks. However, their explanation is based on the assumption that the downstream tasks are *natural tasks*, i.e. tasks that can be reformulated as sentence completion tasks. Their explanation also requires the pretrained language model to perform well for any sentence completion tasks, which is not likely to be true in the real world. Wei et al. (2021) analyze the effect of fine-tuning a pretrained MLM model. Nonetheless, they have stronger assumptions as described in Section A.4. Aghajanyan et al. (2020) show that pretrained models have lower intrinsic dimension, providing a generalization bound based on Arora et al. (2018). However, why pretrained models have lower intrinsic dimension is unknown. Merrill et al. (2021) show that the parameter norm growth during training makes transformer a saturated model, which can be described in terms of formal languages. Empirically, Zhang and Hashimoto (2021) show that the effectiveness of MLM pretraining cannot be explained by formulating the downstream tasks as sentence completion problems. Sinha et al. (2021) find evidence supporting the hypothesis that masked language models benefit from modeling high-order word co-occurrence instead of word order. There are also some theories explaining the efficacy of non-MLM pretraining Lee et al. (2020); Saunshi et al. (2019); Zhang and Stratos (2021).

Many of the previous studies on robust NLP focus on supervised learning (Wang et al., 2021; Utama et al., 2020b,a; Karimi Mahabadi et al., 2020; Chang et al., 2020; He et al., 2019; Sagawa* et al., 2020; Kennedy et al., 2020; Chiang et al., 2020). However, without self-supervised learning, a model can impossibly extrapolate to out-of-distribution data when the domain shifts. Our work also complements previous studies that focus on the bias or robustness of a model generated by the pretraining process (Kumar et al., 2020; Hawkins et al., 2020; Vargas and Cotterell, 2020; Liu et al., 2020; Gonen and Goldberg, 2019; Kurita et al., 2019; Zhao et al., 2019). In this work we investigate the pretraining process itself.

7 Implication and Conclusion

Our results provide possible explanations for some common practices found effective empirically. First, it could explain why continuing pretraining on target dataset is useful (Gururangan et al., 2020). It may be because continuing pretrained models model the distribution of spurious features in the target dataset better. Thus the model can better avoid the simplicity pitfall. Second, it provides reasons for more complex masking policies, such as masking continuous random spans (Joshi et al., 2020). It may improve the robustness to spurious features that contain more than one token. Third, if MLM can alleviate the simplicity bias and help the model to achieve a greater margin, it may also imply that the model has wider optima, explaining the finding in Hao et al. (2019).

In sum, we show a benefit of MLM pretraining, which partly explains its efficacy. We first empirically demonstrate the presence of simplicity bias when the input is discrete. We then theoretically and empirically explain how MLM pretraining can alleviate the problem brought by it. Finally, we close the gap between our theories and real-world practices with experiments on real-world NLP tasks. Our theories reveal a desirable mechanism of MLM pretraining, suggesting that reinforcing this mechanism could be a promising future research direction.

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A Appendix

A.1 Proof of Lemma 1

Proof. Assume that $|\mathcal{X}_2|$ is discrete finite. Since X_2 is discrete and finite, the set $\{P(X_1|x_2)|x_2 \in \mathcal{X}_2\}$ is finite and discrete too. Therefore, the random variable $\Pi \in \{P(X_1|x_2)|x_2 \in \mathcal{X}_2\}$ is also

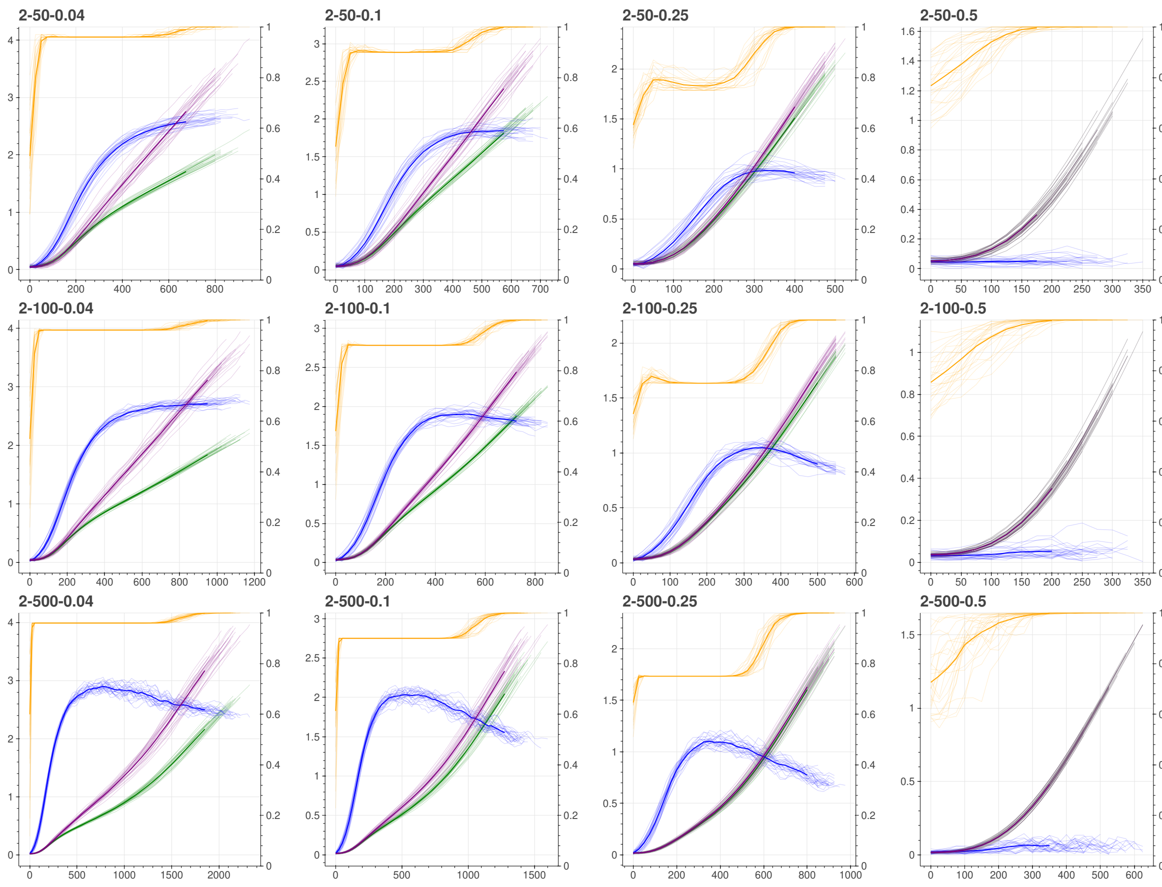

Figure 4: The average weights over the features during training a two-layer model without pretraining. From left to right, $\nu = 0.04, 0.10, 0.25, 0.5$. From top to bottom, $d_2 = 50, 100, 500$. Blue, green, purple curves represent the average weights over features in X_1, X_2, and $\dot{X}_2$ (the middle part of X_2) respectively. The orange curve represents the accuracy.

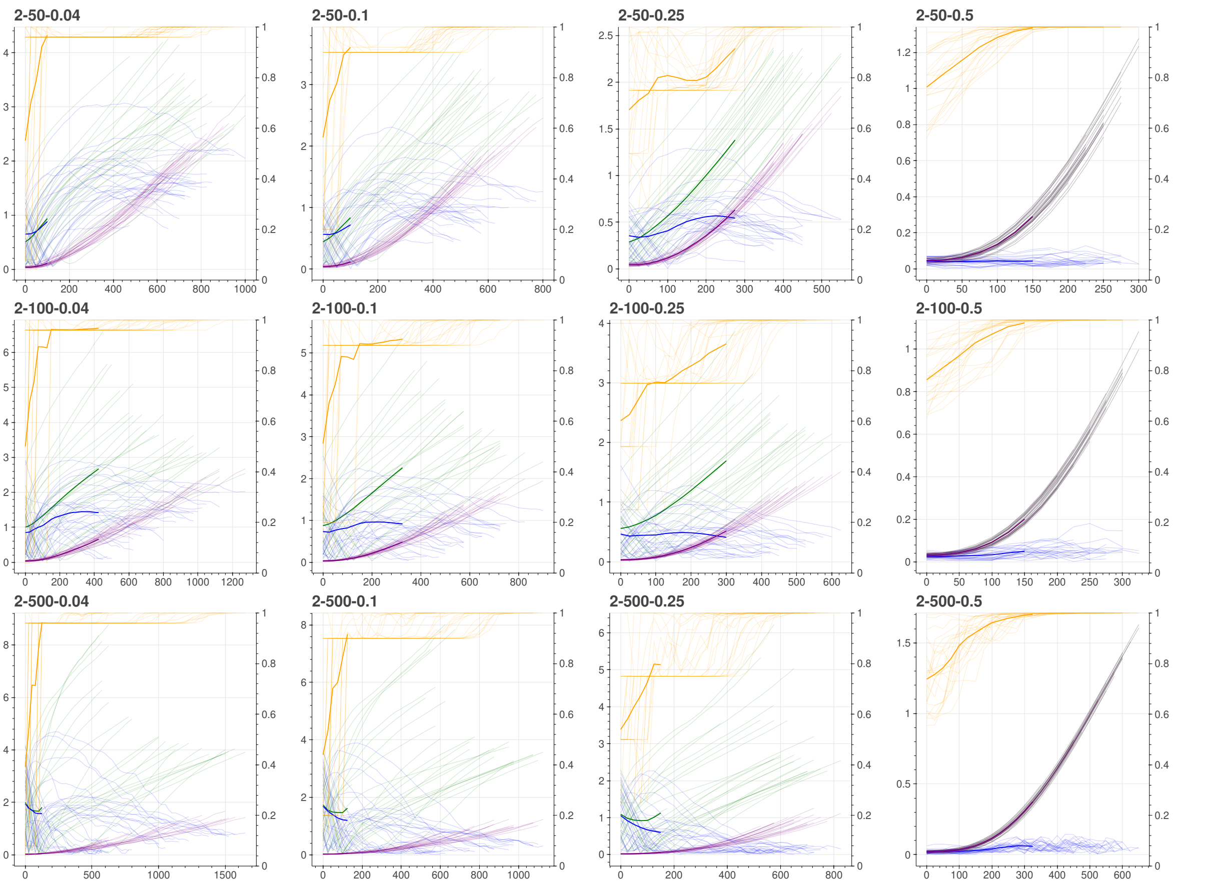

Figure 5: The average weights over the features during training a two-layer model with pretraining. From left to right, $\nu = 0.04, 0.10, 0.25, 0.5$. From top to bottom, $d_2 = 50, 100, 500$. Blue, green, purple curves represent the average weights over features in X_1, X_2, and $\dot{X}_2$ (the middle part of X_2) respectively. The orange curve represents the accuracy.

discrete and finite. So we have

$$\begin{aligned}
&H(X_1|\Pi_1) \\
=&\sum_{x_1,\pi_1} P(X_1,\pi_1)\log P(x_1|\pi_1) \\
=&\sum_{x_1,\pi_1}\sum_{x_2:P(X_1|x_2)=\pi_1} P(x_1,x_2)\log P(x_1|x_2) \\
=&H(X_1|X_2)
\end{aligned}$$

□

Note that the assumption holds when X_2 is a sequence of tokens with bounded length. In practice, the input length of a MLM model is restricted due to the number of position embedding. So the assumption holds in general.

A.2 Proof of Theorem 2

The intuition of the proof is that we compare two classifiers: (1) The one based on X_1, which can be constructed by counting the co-occurrence of X_1 and Y (Eq 10). (2) The one based on Π. The construction of this classifier can be seen as a relaxed version of (1). In (1), we count the occurrence of X_1 based on the observation of X_1. But in (2), we count the occurrence of X_1 based on the likelihood of x_1 for all $x_1 \in \mathcal{X}_1$ (Eq 12).

We then show that (a) the convergence rates of (1) and (2) are asymptotically equal. (b) the converged classifier from (2) is not worse than (1).

To proof Theorem 2, we need a lemma from Gibbs and Su (2002); Paninski (2003) for the convergence rate of empirical measures.

Lemma 2. *Given n samples $x_1, x_2, \cdots, x_n$ of a random variable $X \in \{1, 2, \cdots, m\}$. Let*

$$q_i^{(n)} = \frac{1}{n}\sum_{j=1}^{n} \mathbb{1}[x_j = i]. \tag{8}$$

The expected convergence rate

$$\mathbb{E}\left[D_{KL}\left[q^{(n)} \,\middle\|\, p\right]\right] = O\left(\frac{1}{n}\right), \tag{9}$$

where $p_i = P(X = i)$.

Proof.

$$\begin{aligned}
&\sum_{i=1}^{m} q_i^{(n)} \log \frac{q_i^{(n)}}{p_i} \\
\le&\log\left[\sum_{i=1}^{m} \frac{{q_i^{(n)}}^2}{p_i}\right] \text{ (By concavity of log)} \\
=&\log\left[\sum_{i=1}^{m} \frac{(q_i^{(n)} - p_i)^2}{p_i} + 1\right] \\
\le&\sum_{i=1}^{m} \frac{(q_i^{(n)} - p_i)^2}{p_i}
\end{aligned}$$

$$\mathbb{E}\left[\sum_{i=1}^{m} \frac{(q_i^{(n)} - p_i)^2}{p_i}\right] = O\left(\frac{1}{n}\right)$$

□

Lemma 3. *Let $q^{(a)}, q^{(b)}$ be the empirical distribution estimated by counting n samples following $p^{(a)}, p^{(b)}$. If $D_{KL}\left[p^{(a)} \,\|\, q^{(a)}\right] = O(f(n))$ and $D_{KL}\left[p^{(b)} \,\|\, q^{(b)}\right] = O(f(n))$ for some function $f(n)$ (e.g. $O(\frac{1}{n})$), then $D_{KL}\left[p^{(a)}p^{(b)} \,\|\, q^{(a)}q^{(b)}\right] = O(f)$.*

With these two lemmas, we can prove Theorem 2:

Proof. Proof sketch of Theorem 2: The classifier that maximizes the likelihood of $(x_1^{(1)}, y^{(1)}), (x_1^{(2)}, y^{(2)}), \cdots (x_1^{(n)}, y^{(n)})$ can be attained by counting the co-occurrence of X_1 and Y.

$$\tilde{h}_{X_1}^{(n)}(y|X_1 = x) = \frac{\sum_{i=1}^{n} \mathbb{1}[y^{(i)} = y]\mathbb{1}[x_1^{(i)} = x]}{\sum_{i=1}^{n} \mathbb{1}[x_1^{(i)} = x]} \tag{10}$$

It converges to

$$\tilde{h}_{X_1}^{*}(y|X_1 = x) = P(y|X_1 = x). \tag{11}$$

Based on Π_1, a classifier can be attained by first estimating $P(Y)$ and $P(x_1|y)$ for all x_1 and y:

$$\rho_{y|x_1}^{(n)} = \frac{\sum_{i}^{n} \mathbb{1}[y^{(i)} = y]\pi_{x_1}^{(i)}}{\sum_{i}^{n} \pi_{x_1}^{(i)}}, \tag{12}$$

where $\pi_{x_1}^{(i)} = \Pi(X_1 = x_1^{(n)}|X_2 = x_2^{(n)})$, and then we can construct a classifier

$$\tilde{h}_{\Pi}^{(n)}(y|\pi) = \sum_{x_1} \rho_{y|x_1}^{(n)} \pi_{x_1}. \tag{13}$$

It converges to

$$\tilde{h}^*_{\Pi}(y|\pi) = \sum_{x_1} P(y|x_1)\pi. \tag{14}$$

Based on Lemma 2 and Lemma 3, we have $\mathbb{E}\left[D_{KL}\left[\tilde{h}^{(n)}_{X_1} \,\middle\|\, \tilde{h}^*_{X_1}\right]\right] = O(\frac{1}{n})$ and $\mathbb{E}\left[D_{KL}\left[\tilde{h}^{(n)}_{\Pi} \,\middle\|\, \tilde{h}^*_{\Pi}\right]\right] = O(\frac{1}{n})$.

Then we show that $\tilde{h}^*_{\Pi}(y|\pi)$ is at least as good as $\tilde{h}^*_{X_2}(y|\pi)$ by showing $D_{KL}\left[P(Y|X) \,\middle\|\, \tilde{h}^*_{X_1}(Y|X)\right] \geq D_{KL}\left[P(Y|X) \,\middle\|\, \tilde{h}^*_{\Pi}(Y|X)\right]$ with convexity:

$$\sum_{x_1} P(x_1|x_2) D_{KL}[P(Y|x_2) \parallel P(Y|x_1)] \tag{15}$$

$$\geq D_{KL}\left[P(Y|x_2) \,\middle\|\, \sum_{x_1} P(Y|x_1)P(x_1|x_2)\right]. \tag{16}$$

□

A.3 Elaboration on the Proof of Theorem 4

When X_2 is discrete, we can represent the conditional distribution as a matrix, e.g. $P(X_1|X_2) \in \mathbb{R}^{|\mathcal{X}_1|\times|\mathcal{X}_2|}$, $P(X_1|Y) \in \mathbb{R}^{|\mathcal{X}_1|\times|\mathcal{Y}|}$, $P(Y|X_2) \in \mathbb{R}^{|\mathcal{Y}|\times|\mathcal{X}_2|}$. Therefore, we have

$$P(X_1|X_2) = P(X_1|Y)P(Y|X_2). \tag{17}$$

When the it holds that $\{P(X_1|Y=y)|y \in \mathcal{Y}\}$ are linearly independent, namely columns in $P(X_1|Y)$ are linearly independent, there exists a matrix $A \in \mathbb{R}^{|\mathcal{Y}|\times|\mathcal{X}_1|}$ such that $AP(X_1|Y) = I$. By left multiplying A on the both side of Equation 17, we have

$$P(Y|X_2) = AP(X_1|X_2). \tag{18}$$

The similar technique is used in Lemma 3.1 of Lee et al. (2020).

This implies that Y can predicted based on Π as accurately as predicting based on X_2. Thus, $I(\Pi; Y) \geq I(X_2; Y)$.

A.4 Implementation Details of the Experiments

We pretrain the models until they converge, and choose the checkpoint with the lowest MLM loss on the validation set. For the hate speech detection task, we use the implementation provided by Zhou et al. (2021). Except that we use bert-base-uncased instead of roberta-large, we use the other hyper parameters provided in their script. For the NER task, we use the implementation by Hugging Face [3].

A.5 Details of the Datasets

NER: The size of the training, validation and testing set of Conll-2003 is 14986, 3466 and 2688 respectively. This dataset consists of Reuters news articles. We also use WNUT-17 which is distributed under CC-BY 4.0. The language is English.

Hate Speech Detection: We use the version preprocessed by Zhou et al. (2021). This dataset consists of Twitter comments After filtering out instances without NOI, there are 3491, 672 and 602 instances in the training, validation, testing set respectively. The preprocessed version is distributed under Apache License 2.0. The language is English.

A.6 Computational Budget

Model Size: We use the BERT-base-cased model. The trainable part contains 85M parameters.

Infrastructure: Every experiment can be run with a single NVIDIA GTX 2080Ti GPU. The workstation used for the experiments is equipped with 64G memory.

Computation Time: For the NER task, it takes 90 minutes for a run. For the hate speech detection task, it takes 16 minutes for a run.

[3] https://github.com/huggingface/transformers/blob/master/examples/pytorch/token-classification/run_ner.py