

Repulsive Attention: Rethinking Multi-head Attention as Bayesian Inference

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Abstract

The neural attention mechanism plays an important role in many natural language processing applications. In particular, the use of multi-head attention extends single-head attention by allowing a model to jointly attend information from different perspectives. Without explicit constraining, however, multi-head attention may suffer from *attention collapse*, an issue that makes different heads extract similar attentive features, thus limiting the model’s representation power. In this paper, for the first time, we provide a novel understanding of multi-head attention from a Bayesian perspective. Based on the recently developed particle-optimization sampling techniques, we propose a non-parametric approach that explicitly improves the repulsiveness in multi-head attention and consequently strengthens model’s expressiveness. Remarkably, our Bayesian interpretation provides theoretical inspirations on the not-well-understood questions: why and how one uses multi-head attention. Extensive experiments on various attention models and applications demonstrate that the proposed repulsive attention can improve the learned feature diversity, leading to more informative representations with consistent performance improvement on various tasks.

1 Introduction

Multi-head attention (Vaswani et al., 2017) is an effective module in deep neural networks, with impressive performance gains in many natural-language-processing (NLP) tasks. By extending a single head to multiple paralleled attention heads, the architecture is widely adopted to capture different attentive information and strengthen the expressive power of a model. Lin et al. (2017) applied the idea of multi-heads on self-attention and extract a 2-D matrix instead of a vector to represent different contexts of a sentence. The Transformer (Vaswani et al., 2017) and its variants such

as BERT (Devlin et al., 2019) are influential architectures solely based on multi-head attention, achieving state-of-the-art performance on plenty of NLP tasks. The key of multi-head attention is its ability to jointly attend to information from different representation subspaces at different positions, which results in multiple latent features depicting the input data from different perspectives. However, there are no explicit mechanisms guaranteeing this desired property, leading to potential attention redundancy or attention collapse, which has been observed in previous research (Voita et al., 2019; Kovaleva et al., 2019). Although there exist works by directly adding regularization on loss functions to encourage diversity in multi-head attention (Lin et al., 2017; Li et al., 2018), the underlying working principle has not been well-validated, and performance improvement is limited. Furthermore, an important problem on why and how multi-head attention improves over its single-head counterpart is poorly understood.

In this paper, we provide a novel understanding of multi-head attention from a Bayesian perspective, by adapting the deterministic attention to a stochastic setting. The standard multi-head attention can be understood as a special case of our framework, where attention-parameter updates between heads are independent, instead of sharing a common prior distribution. Based on our framework, attention repulsiveness could then be imposed by performing Bayesian inference on attention parameters with the recently developed particle-optimization sampling methods (Liu and Wang, 2016), which has been shown to be effective in avoiding mode collapse. These methods treat each head as a particle/sample, which is then optimized to approximate a posterior distribution of an attention model. With it, multi heads are enforced to move to the modes in the parameter space to be far from each other, thus improving the repulsive-

ness in multi-head attention and enhancing model’s expressiveness. Our Bayesian interpretation also provides a theoretical understanding on the reason and benefits of applying multi-head attention. Experiments on various attention models demonstrate the effectiveness of our framework.

Our contributions are summarized as follow:

- We provide a new understanding of multi-head attention from a Bayesian perspective, yielding a more principled and flexible interpretation of multi-head attention.
- Based on the recently developed particle-optimization sampling techniques, we propose an algorithm to explicitly encourage repulsiveness in multi-head attention without introducing extra parameters or explicit regularizers. The proposed method can be implemented with an efficient end-to-end training scheme.
- Our Bayesian interpretation provides a theoretical foundation to understand the benefits of multi-head attention, which reveals the existence of an optimal number of attention heads in a specific model.
- We apply our approach on four attention models with a wide range of tasks. Experimental results show that repulsive attention improves the expressiveness of models, and yields consistent performance gains on all the tasks considered.

2 Preliminaries

2.1 Multi-head Attention

The attention mechanism aims at modeling dependencies among elements of a learned representation at different positions. The two commonly used attention functions are additive attention (Lin et al., 2017; Bahdanau et al., 2015) and dot-product attention (Vaswani et al., 2017). We review the popularly used dot-product attention below and defer the additive attention to Appendix A.

Dot-product Attention The multi-head scaled dot-product attention is used in the Transformer model (Vaswani et al., 2017). The attention function for a single head is formulated as mapping a query and a set of key-value pairs to output as

$$\mathbf{A}_i = \text{Softmax}(\mathbf{Q}_i \mathbf{K}_i^T / \sqrt{d_k}), \mathbf{Z}_i = \mathbf{A}_i \mathbf{V}_i \quad (1)$$

$$\text{where } \mathbf{Q}_i = \mathbf{Q} \mathbf{W}_i^Q, \mathbf{K}_i = \mathbf{K} \mathbf{W}_i^K, \mathbf{V}_i = \mathbf{V} \mathbf{W}_i^V$$

$\mathbf{Q}, \mathbf{K}, \mathbf{V}$ are matrices depicting the hidden representation of every word in one sentence (*i.e.* self-attention) or two sentences (*i.e.* inter-attention); d_k is the dimension of key and query; \mathbf{Z}_i is called the attention feature/map of the input sentence from the i -th head; $\{\mathbf{W}_i^Q, \mathbf{W}_i^K, \mathbf{W}_i^V\}$ are the corresponding learnable attention parameters. The M -head attention projects the queries, keys and values into M subspaces with different learnable linear projections. These attention functions are performed in parallel and are concatenated at last, resulting in a final latent representation:

$$\begin{aligned} \text{Multi-head}(\mathbf{Q}, \mathbf{K}, \mathbf{V}) &= \mathbf{Z} \mathbf{W}^O, \text{ with} \\ \mathbf{Z} &= \text{Concat}(\mathbf{Z}_1, \dots, \mathbf{Z}_M) \end{aligned} \quad (2)$$

2.2 Particle-Optimization Sampling

Particle-optimization sampling is a recently developed Bayesian sampling technique that interactively transports a set of particles/samples to a target distribution p by minimizing the KL divergence between the particle density and the target p . In our case, p would be a posterior distribution, $p(\boldsymbol{\theta}|\mathcal{D}) \propto \exp(-U(\boldsymbol{\theta}))$, of the parameter $\boldsymbol{\theta} \in \mathbb{R}^d$, defined over an observed dataset $\mathcal{D} = \{D_k\}_{k=1}^N$. Here $U(\boldsymbol{\theta}) \triangleq -\log p(\mathcal{D}|\boldsymbol{\theta}) - \log p_0(\boldsymbol{\theta}) = -\sum_{k=1}^N \log p(D_k|\boldsymbol{\theta}) - \log p_0(\boldsymbol{\theta})$ is called the potential energy with p_0 a prior over $\boldsymbol{\theta}$. In our case, the model parameter $\boldsymbol{\theta}$ could be one or several of the attention parameters such as \mathbf{W}_i^Q . For simplicity, we will stick to $\boldsymbol{\theta}$ in the presentation. In particle-optimization sampling, a total of M particles $\{\boldsymbol{\theta}_i^{(i)}\}_{i=1}^M$ are updated iteratively to approximate $p(\boldsymbol{\theta}|\mathcal{D})$. In this paper, we use two representative algorithms, the Stein Variational Gradient Descent (SVGD) and the Stochastic Particle-Optimization Sampling (SPOS), for sampling.

SVGD In SVGD (Liu and Wang, 2016), the i -th particle in the $(\ell+1)$ -th iteration is updated with stepsize $\epsilon_{\ell+1}$ as

$$\boldsymbol{\theta}_{\ell+1}^{(i)} = \boldsymbol{\theta}_\ell^{(i)} + \epsilon_{\ell+1} \phi(\boldsymbol{\theta}_\ell^{(i)}) \quad (3)$$

$$\begin{aligned} \phi(\boldsymbol{\theta}_\ell^{(i)}) &= \frac{1}{M} \sum_{j=1}^M [-\kappa(\boldsymbol{\theta}_\ell^{(j)}, \boldsymbol{\theta}_\ell^{(i)}) \nabla_{\boldsymbol{\theta}_\ell^{(j)}} U(\boldsymbol{\theta}_\ell^{(j)}) \\ &\quad + \nabla_{\boldsymbol{\theta}_\ell^{(j)}} \kappa(\boldsymbol{\theta}_\ell^{(j)}, \boldsymbol{\theta}_\ell^{(i)})] \end{aligned} \quad (4)$$

where $\kappa(\cdot, \cdot)$ is a positive definite kernel (*e.g.*, RBF kernel). The two terms in ϕ play different roles: the first term drives the particles towards high density regions of $p(\boldsymbol{\theta}|\mathcal{D})$; whereas the second term acts as

a repulsive force that prevents all the particles from collapsing together into local modes of $p(\theta|\mathcal{D})$.

SPOS Though obtaining significant empirical success, under certain conditions, SVGD experiences a theoretical pitfall, where particles tend to collapse. To overcome this, [Zhang et al. \(2018\)](#) generalize SVGD to a stochastic setting by injecting random noise into particle updates. The update rule for particles $\theta_\ell^{(i)}$ is

$$\begin{aligned}\phi(\theta_\ell^{(i)}) &= \frac{1}{M} \sum_{j=1}^M [-\kappa(\theta_\ell^{(j)}, \theta_\ell^{(i)}) \nabla_{\theta_\ell^{(j)}} U(\theta_\ell^{(j)}) + \\ &\quad \nabla_{\theta_\ell^{(j)}} \kappa(\theta_\ell^{(j)}, \theta_\ell^{(i)})] - \beta^{-1} \nabla_{\theta_\ell^{(i)}} U(\theta_\ell^{(i)}) + \sqrt{2\beta^{-1}\epsilon_\ell^{-1}} \xi_\ell^{(i)}\end{aligned}\quad (5)$$

where $\beta > 0$ is a hyperparameter, $\xi_\ell^{(i)} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ is the injected random Gaussian noise to enhance the ability of escaping local modes, leading to better ergodic properties compared to standard SVGD.

3 A Bayesian-Inference Perspective of Multi-Head Attention

In this section, we interpret multi-head attention as Bayesian inference of latent representation via particle-optimization sampling. We denote x and z as the input and output (latent representation) of the attention model, respectively. The single-head attention can be written as a deterministic mapping $z = f_{att}(x; \theta)$, with θ the parameter of the mapping. Standard multi-head attention defines multiple parallel attention mappings, each endowed with independent parameters. The attention features are finally aggregated via a function $g(\cdot)$ as

$$z = g(z_1, \dots, z_M), \quad z_i = f_{att}(x; \theta_i). \quad (6)$$

Next, we generalize (6) as a Bayesian inference problem for the latent representation z .

Attention as Bayesian Inference We first generalize the deterministic transformation, $z = f_{att}(x; \theta)$, to a stochastic generative process as:

$$\theta \sim p(\theta|\mathcal{D}), \quad z = f_{att}(x; \theta),$$

where a sample of the posterior of the global attention parameter θ , $p(\theta|\mathcal{D}) \propto p(\mathcal{D}|\theta)p(\theta)$, is used as the parameter when generating the latent attention feature z . Bayesian inference for attention then computes the predictive distribution $p(z|x, \mathcal{D})$ of the attentive latent representation z for a new input x given the training data \mathcal{D} by $p(z|x, \mathcal{D}) = \int \delta_{f_{att}(x; \theta)}(z) p(\theta|\mathcal{D}) d\theta$, where

$\delta_z(\cdot)$ is the delta function with point mass at z . To enable efficient evaluation of the integral, we adopt Bayesian sampling for approximation, *i.e.*, $p(z|x, \mathcal{D})$ is approximated by a set of M samples/particles initialized from $p(\theta|\mathcal{D})$, leading to the following generative process:

$$\begin{aligned}z &= g(z_1, \dots, z_M) \\ z_i &= f_{att}(x; \theta_i), \quad \text{with } \theta_i \sim p(\theta|\mathcal{D})\end{aligned}\quad (7)$$

The above formulation defines a principled version of multi-head attention from a Bayesian view. One can see that (7) reduces to the standard multi-head attention if all θ_i are treated independently without sharing the common parameter distribution $p(\theta|\mathcal{D})$. In other words, our reformulation of multi-head attention is a stochastic generative process, thus is more general. Furthermore, efficient end-to-end learning can be performed by conducting repulsive Bayesian sampling for all parameters $\{\theta_i\}_{i=1}^M$, which consequently could diversify the attention features $\{z_i\}_{i=1}^M$.

4 Repulsive Attention Optimization

The Bayesian multi-head attention in (7) further inspires us to develop the repulsive attention. The idea is to learn to generate repulsive samples from the posterior $p(\theta|\mathcal{D})$. We propose to adopt the particle-optimization sampling methods, which could explicitly encourage repulsiveness between samples. In our algorithm, the parameter of $p(z|x; \theta)$ for each head is considered as one particle. Following the particle-optimization rules, M heads $\{\theta_i\}_{i=1}^M$ are updated iteratively to approximate the posterior distribution of attention parameter $p(\theta|\mathcal{D})$.

4.1 Learning Repulsive Multi-head Attention

We propose to learning repulsive attention by replacing the standard updates of attention parameters via stochastic gradient descent (SGD) with particle-optimization sampling methods while keeping the architecture of the multi-head attention unchanged. This procedure forms an efficient end-to-end training scheme similar to standard attention learning. To be specific, in standard multi-head attention, the parameter of every head is updated independently according to the respective gradient of a loss function. To achieve repulsive multi-head attention, we follow the particle-optimization sampling update rule (*e.g.* (3) and (4)) to update the parameter of every head while keeping the update

for the remaining parameters via SGD unchanged. Equations (4) and (5) can be viewed as modified gradients with explicit repulsive force and can be integrated into any optimizer, *e.g.*, Adam (Kingma and Ba, 2015). Note that $\nabla_{\theta_\ell^{(i)}} U(\theta_\ell^{(i)})$ equals to the gradient of $\theta_\ell^{(i)}$ in standard multi-head attention when the negative log-likelihood is used as the loss function and the prior of $\theta^{(i)}$ is assumed to be uniform. The learning algorithm is illustrated in Algorithm 1. In practice, the update of M heads can be performed in parallel with efficient matrix operations.

Algorithm 1 Repulsive Multi-head Attention

Input: Initialized M -head attention model \mathcal{A} with attention parameters $\Theta_0 = \{\theta_i\}_{i=1}^M$ and other parameters Ω_0 ; Training data $\mathcal{D} = \{D_k\}_{k=1}^N = \{(\mathbf{x}_k, y_k)\}_{k=1}^N$;

Output: Optimized attention model with learned parameters $\hat{\Theta}$ and $\hat{\Omega}$;

Train:

```

for iteration  $\ell$  do
    forward:  $\hat{y}_k = \mathcal{A}(\mathbf{x}_k; \Theta_\ell, \Omega_\ell), \forall k$ ;
    calculate loss:  $\mathcal{L}(\{\hat{y}_k\}, \{y_k\})$ ;
    backward and calculate gradients:
    gradient of  $\Omega_\ell$ :  $\varphi(\Omega_\ell) \leftarrow \nabla_{\Omega_\ell} \mathcal{L}$ 
    for attention head  $i$  do
        calculate  $\phi(\theta_\ell^{(i)})$  with Eq (4) or (5);
        gradient of  $\theta_\ell^{(i)}$ :  $\varphi(\theta_\ell^{(i)}) \leftarrow \epsilon_\ell \phi(\theta_\ell^{(i)})$ ;
    end for
    update parameters:
     $\Omega_{\ell+1} \leftarrow \text{Optimizer}(\Omega_\ell, \varphi(\Omega_\ell))$ 
     $\Theta_{\ell+1} \leftarrow \text{Optimizer}(\Theta_\ell, \varphi(\Theta_\ell))$ 
end for

```

4.2 In-depth Analysis

Why Multi-head Attention? Our Bayesian interpretation of the attention mechanism naturally provides an answer to the question of why one needs multi-head attention. By treating each head as one sample, adopting multiple heads means using more samples to approximate an underlying posterior distribution. The question comes to should one use more heads (samples). Intuitively this seems to be true because more samples typically make more accurate approximations. However, this could not be the case in practice. The reason might be two-fold: *i) Overfitting*: Learning with a limited amount of data could easily cause overfitting, thus requiring a smaller model (less at-

tention heads); *ii) Numerical error*: Our proposed method to update samples (attention-head parameters) is essentially a discrete numerical method of the corresponding continuous-time partial differential equation, *i.e.*, the samples are not exact samples from the target distribution. Thanks to the recently developed theory for particle-optimization sampling (Zhang et al., 2018), one can conclude that more heads could accumulate more numerical errors, leading to performance deterioration. More formally, when using particles to approximate a target posterior distribution, there exists a gap (approximation error) between the particle distribution and the true distribution (Zhang et al., 2018). This approximation error, when applied to our setting, approximately scales in the order of $O(\frac{1}{\sqrt{M}} + M\epsilon_0^{1/2} + e^{-\sum \epsilon_\ell \epsilon_\ell})$. Please refer to Theorem 10 in (Zhang et al., 2018) for a formal description.

How Many Heads are Enough? The above error bound suggests that there is a trade-off between approximation accuracy and the number of heads M . Specifically, we have *i)* when M is small, the term $\frac{1}{\sqrt{M}}$ in the bound would dominate, leading to decreasing errors (increasing performance) with increasing M ; *ii)* when M is large enough, the term $M\epsilon_0^{1/2}$ dominates, suggesting that larger M could actually increase the approximation error (decreased performance). These phenomena are consistent with our experimental results. We note that an exact form of the optimal M is not available due to a number of unknown constants (omitted in the big-O notation). Therefore, one should seek other ways such as cross-validation to choose a good M in practice. Our argument also aligns with recent research, which found that more heads do not necessarily lead to better performance (Michel et al., 2019).

5 Experiments

We demonstrate the effectiveness of our method with representative multi-head attention models on a broad range of tasks including sentence classification, machine translation, language modeling and text generation. This section summarizes key results on different models. More detailed analysis and extra experiments are deferred to the appendix. To apply our approach, only the learning method of multi-head attention is adapted.

the food was amazing and worth the dip in the pocketbook . a downfall was the atmosphere felt like a cafeteria . service was passing .
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(a) detailed attentions

the food was amazing and worth the dip in the pocketbook . a downfall was the atmosphere felt like a cafeteria . service was passing .

(c) standard multi-head attention

the food was amazing and worth the dip in the pocketbook . a downfall was the atmosphere felt like a cafeteria . service was passing .

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(b) detailed attentions

the food was amazing and worth the dip in the pocketbook . a downfall was the atmosphere felt like a cafeteria . service was passing .

(d) repulsive multi-head attention

Figure 1: Attention heatmaps of a 4-star Yelp review. Results on the left is from the standard multi-head attention, and the result on the right is from our repulsive multi-head attention. (a) and (b) shows detailed attention maps taken by 5 out of 30 rows of the matrix embedding, while (c) and (d) shows the overall attention by summing up all 30 attention weight vectors.

Models	Acc(%)	Dist
Age		
BiLSTM + MA	81.47	0.129
BiLSTM + MA + R	81.30	0.178
BiLSTM + RMA (SVGD)	81.82	0.492
BiLSTM + RMA (SPOS)	82.55	0.461
Yelp		
BiLSTM + MA	69.3	0.246
BiLSTM + MA + R	70.2	0.536
BiLSTM + RMA (SVGD)	71.2	1.602
BiLSTM + RMA (SPOS)	71.7	1.655
SNLI		
BiLSTM + MA	83.79	1.293
BiLSTM + MA + R	84.55	1.606
BiLSTM + RMA (SVGD)	84.58	1.688
BiLSTM + RMA (SPOS)	84.76	1.370

Table 1: Performance (accuracy) comparison on Age, Yelp and SNLI dataset. Dist: the average 2-norm distance between each pair of the latent representation encoded from different heads on test set. MA: standard multi-head attention. RMA: proposed repulsive multi-head attention. R: regularization approach.

5.1 Self-attentive Sentence Classification

Model & Baselines We first apply our method to the self-attentive sentence classification model (Lin et al., 2017) which combines BiLSTM with additive attention to learn the sentence embedding and then does classification on it. We compare our method with the one using the standard multi-head attention (BiLSTM + MA) and the one applying the Frobenius regularization (BiLSTM + MA + R) on it to introduce diversity as in Lin et al. (2017).

Tasks & Datasets Following Lin et al. (2017), three sentence classification tasks including author profiling, sentiment analysis, and textual entailment are evaluated on the Age, Yelp, and SNLI datasets respectively.

Results As shown in Table 1, with the proposed repulsive multi-head attention, the model achieves higher accuracy on all three tasks. Especially on the sentiment analysis task which often contains multiple aspects in one sentence. Our methods also outperform the regularization method proposed in Lin et al. (2017). With different particle-optimization rules, SPOS is able to achieve better performance due to its extra advance discussed by Zhang et al. (2018). We further evaluate the diversity of multiple heads by calculating the average distance between each pair of latent representations. Results show that our methods indeed enforce heads to be more diverse, compared with the standard multi-head attention. The less diverse of the regularization-based method also indicates the validness of our argument in Appendix C.6.

Repulsive-attention visualization We further visualize attention maps in the learned sentence embedding space in Figure 1. It is interesting to see attention collapse indeed happens in the standard multi-head attention, where almost all heads focus on one single factor “amazing”. On the contrary, the proposed method is able to capture multiple key factors in the review that are strong indicators of the sentiment behind the sentence. For example, “downfall” and “service was passing” are key factors for this 4-star review captured by our repulsive

Models	BLEU	Time
IWSLT14 De-En		
Transformer-small-MA	34.4	1
Transformer-small-MA + R	34.9	1.29
Transformer-small-RMA	35.2	1.13
WMT14 En-De		
Transformer-base-MA	27.3	1
Transformer-base-MA + R	28.2	1.35
Transformer-big-MA	28.4	-
Transformer-base-RMA	28.4	1.18

Table 2: Translation Performance on IWSLT14 De-En and WMT14 En-De Datasets. MA: standard multi-head attention. RMA: proposed repulsive multi-head attention. R: regularization approach. Time: relative training time of every step versus MA.

multi-head attention, which are missed by the standard attention. The full attention heatmaps of all 30 heads and more examples are in Appendix D.

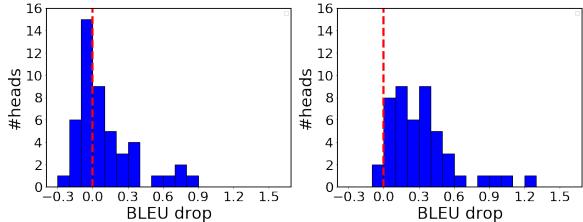
5.2 Transformer-based Neural Translation

Model & Baselines The Transformer (Vaswani et al., 2017) is a representative multi-head attention based model. We apply the proposed repulsive multi-head attention (RMA) on it and compare our method with the original one (MA) and the disagreement regularization method (R) (Li et al., 2018) which encourages the diversity in attention by a cosine similarity penalty on attention outputs.

Tasks & Datasets Following Vaswani et al. (2017), we apply Transformer for machine translation, with two standard translation datasets: the IWSLT14 German-to-English (De-En) dataset, and the WMT14 English-to-German (En-De) dataset.

Results Results are presented in Table 2. With the repulsive multi-head attention, Transformer models achieve noticeable improvement on the BLEU score on both datasets, compared with both baselines. It is also encouraging to see that the Transformer-base-RMA with a much smaller model achieves comparable performance as Transformer-big. As for training time, our approach takes slightly more time than the baseline, but is much more efficient than the regularization approach. A more detailed analysis of the computational complexity is provided in Appendix B.3.

Which attention module to be diversified? We conduct extra experiments on Transformer-small to investigate which attention module benefits most from the repulsiveness. Results (see Appendix C.3) suggest that diversifying different attention module



(a) Transformer-base-MA (b) Transformer-base-RMA

Figure 2: Distribution of heads by performance drop after masking at test time. The redundancy of heads in RMA is much less.

benefits differently. Remarkably, only diversifying the attention in the first layer is able to achieve comparable performance to the case of diversifying attention in all layers, with little computational time increased. This finding suggests that the repulsiveness in the first layer’s attention plays an important role for modelling language.

Redundancy in heads The redundancy problem in attention has been observed in recent works (Michel et al., 2019), that a large percentage of attention heads can be removed at test time without significantly impacting performance. Following Michel et al. (2019), we analysis the redundancy in Transformer by ablating each head at testing and evaluating the performance drop. The more drops, the more important of the head. Figure 2 shows that the majority of heads in standard multi-head attention are redundant for the performance is comparable before and after masking. However, the repulsive attention largely alleviates the redundancy. More interestingly, there are a lot of counter-intuitive cases in standard attention: removing a head results in an increase in performance. However, this does not seem to happen in repulsive attention model, indicating better leveraging of the superior expressiveness of multi-head mechanism.

5.3 Language Representation Learning

Model ELECTRA (Clark et al., 2020) is an efficient approach to self-supervised language representation learning. It consists of two networks, *Generator* and *Discriminator*, both of which are parameterized by Transformers. The pre-trained Discriminator is used in various downstream tasks via fine-tuning. We apply the proposed repulsive multi-head attention to ELECTRA (small setting) in the pre-training stage. We only make the first layer attention of Discriminator to be repulsive, according to the finding in Section 5.2 that the di-

Pre-training Data	Model	Prams	CoLA	SST	MRPC	STS	QQP	MNLI	QNLI	RTE	Avg.
Wikipedia + BooksCorpus	TinyBERT	14.5M	51.1	93.1	82.6	83.7	89.1	84.6	90.4	70.0	80.6
	MobileBERT	25.3M	51.1	92.6	84.5	84.8	88.3	84.3	91.6	70.4	81.0
	GPT	117M	45.4	91.3	75.7	80.0	88.5	82.1	88.1	56.0	75.9
	BERT-Base	110M	52.1	93.5	84.8	85.8	89.2	84.6	90.5	66.4	80.9
	ELECTRA	14M	54.6	89.1	83.7	80.3	88.0	79.7	87.7	60.8	78.0
OpenWebText	ELECTRA + RMA	14M 14M	56.2 59.4	88.3 87.1	87.5 87.9	86.8 87.0	88.1 88.6	78.6 79.3	87.4 87.8	67.3 / 71.4 64.9 / 73.1	80.0 / 80.5 80.3 / 81.3

Table 3: Results on the GLUE test set. For RMA, repulsive attention is only applied to pre-training. For RTE, the left value is fine-tuned from pre-trained models, the right value is from intermediate task training.

versity in the first attention layer of Transformer benefits the most.

Tasks & Dataset We train ELECTRA models on OpenWebText Corpus due to the data used in Clark et al. (2020) is not publicly available. The pretrained models are then fine-tuned and evaluated on the General Language Understanding Evaluation (GLUE) (Wang et al., 2019) benchmark.

Results Results are shown in Table 3. For each task, we perform single-task fine-tuning 50 trails, and report the averaged results. The training time with and without repulsive attention is almost the same. It shows that repulsive attention improves the baseline results (Clark et al., 2020) in seven out of eight tasks on GLUE, and the gains are larger especially on MNLI (the largest dataset on GLUE) and CoLA . This suggests that repulsive attention can yield better language representations. Following Phang et al. (2018), we use intermediate task training for RTE, which first fine-tunes pre-trained model on MNLI, then continuously fine-tuned it on RTE. The repulsive attention outperform the baseline method by a large margin in this setting. This is probably because the the repulsive attention particularly favor large data variability (e.g., MNLI dataset), where different aspects of data can be uniquely represented in different heads.

5.4 Graph-to-Text Generation

Model & Baselines GraphWriter (Koncel-Kedziorski et al., 2019) is a knowledge-graph-to-text model, which aims at generating coherent multi-sentence abstract given a knowledge graph and a title. There is a Transformer-style encoder defined with graph attention modules (Velickovic et al., 2018) that could also be easily adapted to our method. We compare our method with the original one that has the standard multi-head attention, and the one with the cosine similarity regularization on attention parameters in encoder layers.

Metrics	GW	+ R	+ RMA
BLEU-1	42.56	42.25	45.60
BLEU-2	27.64	27.98	29.96
BLEU-3	19.27	19.77	21.07
BLEU-4	13.75	14.21	15.12
METEOR	18.11	18.61	19.52
ROUGE-1	35.80	37.24	38.23
ROUGE-2	16.83	17.78	18.39
ROUGE-L	27.21	26.90	28.55

Table 4: Automatic evaluations of generation systems on test set of AGENDA.

	Win	Lose	Tie
Structure	51%	12%	37%
Informativeness	66%	13%	21%
Grammar	37%	17%	46%
Overall	65%	14%	21%

Table 5: Human judgments of GraphWriter with and without repulsive attention.

Tasks & Datasets & Metrics Experiments are conducted on the Abstract GENeration DATaset (AGENDA) (Koncel-Kedziorski et al., 2019), a dataset of knowledge graphs paired with scientific abstracts. We evaluate the quality of abstracts with 3 major metrics: BLEU (uni-gram to 4-gram BLEU) (Papineni et al., 2002), METEOR (Banerjee and Lavie, 2005), ROUGE (Lin and Hovy, 2003). In ROUGE, the unigram and bigram overlap (ROUGE-1 and ROUGE-2) are a proxy for assessing informativeness and the longest common subsequence (ROUGE-L) represents fluency.

Results The results are shown in Table 4. The GraphWriter model with repulsive multi-head attention significantly outperforms the original model and regularization approach in all metrics. Especially, the higher recall score in ROUGE shows that there are more N-grams across the reference abstracts that can be found in the generated abstracts. Similar observations are noticed when analyzing the generated examples in detail (an example is illustrated in Appendix E). Koncel-Kedziorski et al.

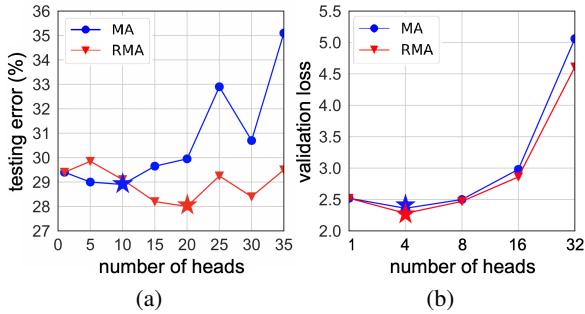


Figure 3: Demonstration on performance variant with number of heads. (a) Testing error of the self-attentive sentence classification model on Yelp dataset. (b) Negative log likelihood loss of Transformer-small on IWSLT14 De-En dataset.

(2019) pointed out one limitation of their model, which is 40% of entities in the knowledge graphs do not appear in the generated text. With the repulsive attention, remarkably, the GraphWriter model is observed to perform much better with a 10% improvement on the knowledge graph coverage and fewer repeat clauses.

Human Evaluation To further illustrate the improvement of using diverse attention, we conduct human evaluation. Following Koncel-Kedziorski et al. (2019), we give 50 test datapoints to experts (5 computer science students) and ask them to provide per-criterion judgments for the generated abstracts. Comparisons of the two methods from 4 aspects are shown in Table 5. The human judgment indicates that the repulsive attention improves both the structure and informativeness of generated abstracts significantly, which is consistent with the automatic evaluation and our observations.

5.5 On the Number of Attention Heads

Our analysis in Section 4.2 suggests the existence of the optimal number of attention heads. To verify this, we further conduct experiments on sentence classification and translation tasks by varying the number of attention heads in models. The results are shown in Figure 3. The model error/loss first decreases then increases w.r.t. M , the number of attention heads. The optimal M are around 20 and 4 for the sentiment analysis and the Transformer, respectively. Interestingly, the Transformer degrades quickly as the number of heads increases. This might because the constant corresponding to the $O(M\epsilon_0)$ term in the bound is too large, making this term quickly dominate with increasing M . Furthermore, it is also observed that the standard multi-

head attention follows the same trend, but performs much worse and is more sensitive to the M . This indicates the benefit of Bayesian modeling, which could usually stabilize a model better.

6 Related Work

We provide a first explanation of multi-head attention from a Bayesian perspective, and propose particle-optimization sampling for repulsive attention. Most previous works aim at improving attention diversity with regularization-based methods, e.g., the Frobenius regularization on attention weights in Lin et al. (2017) and the cosine similarity regularization on attention outputs in Li et al. (2018). These works focus on a particular model and the underlying working principle has not been well-validated. Our approach is a principled one that is more interpretable and widely applicable.

The attention collapse belongs to a feature-overlapping problem, which also happens in other areas. Some works tackle this problem by changing architectures, for example ResNet (He et al., 2016) and DenseNet (Huang et al., 2017) implicitly reduce feature correlations by summing or concatenating activation from previous layers. There are also works done by altering the training method as what we do. Han et al. (2017) adopt the dropout mechanism and propose a dense-sparse-dense training flow, for regularizing deep neural networks. Later, Prakash et al. (2019) attempted addressing the unnecessary overlap in features captured by image filters with pruning-restoring scheme in training. To our knowledge, we are the first to tackle the attention-feature overlap problem from a Bayesian view with a principled interpretation.

7 Conclusion

We propose a principled way of understanding multi-head attention from a Bayesian perspective. We apply particle-optimization sampling to train repulsive multi-head attention without additional parameters nor explicit regularizers. Our Bayesian framework explains the long-standing question of why and how multi-head attention affects model performance. Extensive experimental results on representative attention models demonstrate that our approach can significantly improve the diversity in multi-head attention, resulting in more expressiveness attention models with performance improvement on a wide range of tasks.

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A Additive Attention

First proposed by (Bahdanau et al., 2015), additive attention uses a one-hidden layer feed-forward network to calculate the attention alignment. We use the attention function in Lin et al. (2017), which is also a self-attention, as an example. It aims at extracting the latent representation of a sentence. The single-head attention function is:

$$\mathbf{a} = \text{Softmax}(\mathbf{v}^\top \tanh(\mathbf{W}\mathbf{H}^\top)), \mathbf{z} = \mathbf{a}\mathbf{H} \quad (8)$$

where $\mathbf{H} \in \mathbb{R}^{n \times d}$ is the hidden state matrix of a sentence with n words, every word is embedded in a d dimensional vector. $\mathbf{v} \in \mathbb{R}^{1 \times n}$ is the normalized alignment score vector for each word. $\mathbf{W} \in \mathbb{R}^{d_a \times d}$ and $\mathbf{v} \in \mathbb{R}^{d_a \times 1}$ are attention parameters. The final sentence representation vector \mathbf{z} is a weighted sum of words' hidden states weighted by attention vector. In order to capture overall semantics of the sentence instead of a specific component, multi-head attention could be applied as

$$\mathbf{A} = \text{Softmax}(\mathbf{V}^\top \tanh(\mathbf{W}\mathbf{H}^\top)), \mathbf{Z} = \mathbf{A}\mathbf{H} \quad (9)$$

where $\mathbf{V} \in \mathbb{R}^{d_a \times M}$ is the matrix performs M heads, $\mathbf{A} \in \mathbb{R}^{M \times n}$ is the M -head attention matrix and $\mathbf{Z} \in \mathbb{R}^{M \times d}$ is the resulting sentence representation matrix contains semantics from multiple aspects.

B Additional Experimental Details and Results

B.1 Cyberbullying Detection

Tasks & Datasets To further assess the effectiveness of our model, we apply it on abusive-comment detection task. Two datasets from Twitter and Wikipedia talk pages are used. Our goal is to distinguish bullying comments from non-bullying ones.

Baselines We have tested several baseline models and found the following most effective: (1) BiLSTM + MA: A sentence embedding model with BiLSTM and standard multi-head attention (MA). (2) CNN: A classical temporal Convolutional Neural Networks to process text. (3) NBLR: The Naive Bayes Logistic Regression.

Main Results To evaluate the capability of our model to detect attack annotation comments, several metrics including receiver operating characteristic curve (AUC@ROC) and precision-recall curve (AUC@PR) are adopted. Compared to other metrics such as F1 score and Matthews correlation coefficient ($\text{MCC} \in [-1, 1]$, 1 for perfect prediction (Matthews, 1975)), AUC@PR shows a more informative picture of a model's performance, especially when the datasets are highly skewed, as is our case (Davis and Goadrich, 2006). Table 6 shows the results. Similar to sentence classification tasks, with repulsive attention, our model performs better than all the baselines.

Models	AUC@ROC	AUC@PR	MCC	F1 Score
Twitter				
CNN	0.8247	0.7174	0.5041	0.6264
NBLR	0.9105	0.8454	0.6280	0.7116
BiLSTM + MA	0.9020	0.7999	0.6391	0.7403
BiLSTM + RMA	0.9275	0.8552	0.6832	0.7819
Wikipedia				
CNN	0.9526	0.8202	0.7058	0.7304
NBLR	0.9687	0.8674	0.7389	0.7533
BiLSTM + MA	0.9720	0.8642	0.7506	0.7790
BiLSTM + RMA	0.9732	0.8713	0.7646	0.7896

Table 6: Performance comparison between different Multi-head attention mechanism on Wikipedia and Twitter for baseline models and ours. RMA: the proposed repulsive multi-head attention via SVGD. Diversed attention with SPOS obtains comparable results in this case, thus are not included.

B.2 Experimental Details

For our approach, RBF kernel $\kappa(x, y) = \exp(-\frac{1}{h}\|x - y\|_2^2)$ with the bandwidth $h = med^2 / \log M$ is used as the kernel function, where med denotes the median of the pairwise distance between current particles. The prior distribution of attention parameters is assumed to be uniform. We find that adding an repulsive weight before the repulsive term (i.e. the second term in Eq. 4) in particle-optimization update rules could help adjusting the degree of diversity in attention and achieving better performance. In our experiments, we adopt this trick and use the hyper-parameter α to denote the repulsive weight. Since our method only modifies the learning process of attention, all models and settings in our experiments kept the same with the corresponding previous work unless stated otherwise.

B.2.1 Self-attentive Sentence Classification

Dataset Three tasks are conducted on three public sentence classification datasets. *Author profiling* (Age dataset¹) is to predict the age range of the user by giving their tweets. *Sentiment analysis* (Yelp dataset²) is to predict the number of stars the user assigned to by analysis their reviews. *Textual entailment* (SNLI dataset³) is to tell whether the semantics in the two sentences are entailment or contradiction or neutral. Following Lin et al. (2017), the train / validate / test split of Age is 68485 / 4000 / 4000, Yelp is 500K / 2000 / 2000, SNLI is 550K / 10K / 10K.

Experimental settings We implement the standard multi-head attention model in Lin et al. (2017) following the settings in it except that we use Spacy toolkit⁴ as the tokenizer and GloVe⁵ (GloVe 840B 300D) as the pre-trained word embedding. For repulsive multi-head attention learning, we keep all settings the same with the standard one (Lin et al., 2017). Hyper-parameters ϵ , α and β in particle-optimization rules are manually tuned for each task. We train and evaluate all the models with 10 random seeds and compare their average performance. Models are trained on one TITAN Xp GPU.

B.2.2 Cyberbullying Detection

Dataset Two cyberbullying detection datasets⁶ are used in this experiment. The train / validate / test split of Twitter is 9572 / 3254 / 3254, Wikipedia is 69987 / 22952 / 22952. Table 7 shows more detailss.

Source	# Abusive	# Clean	# Total	% Abusive
Wikipedia	13590	102274	115864	11.7%
Twitter	5054	11036	16090	31.4 %

Table 7: Static description of cyberbullying detection datasets

Experimental settings We adopt similar settings to sentence classification tasks in our implementation, except some minor differences. For repulsive multi-head attention, we use grid search to determine stepsize ϵ and repulsive weight α . The number of attention heads is set to 15. The size of the hidden units and embeddings is 300. The model is trained on one TITAN Xp GPU.

B.2.3 Transformer-based Neural Translation

Dataset IWSLT14 German-to-English (De-En) dataset contains 153K / 7K / 7K sentence pairs. WMT14 English-to-German (En-De) dataset contains about 4.5 million training sentence pairs and uses newstest2013 dataset as the validation set, newstest2014 dataset as the test set. Data and the processing scripts could be found here⁷.

¹<https://pan.webis.de/clef16/pan16-web/author-profiling.html>

²<https://www.yelp.com/dataset/download>

³<https://nlp.stanford.edu/projects/snli/>

⁴<https://spacy.io/>

⁵<https://nlp.stanford.edu/projects/glove/>

⁶Dataset can be obtained via <https://github.com/sweta20/Detecting-Cyberbullying-Across-SMPs>

⁷<https://github.com/pytorch/fairseq/tree/v0.6.0/examples/translation>

Experimental settings Our implementation is based on the open-sourced `fairseq`⁸ (Ott et al., 2019). We follow the settings in Vaswani et al. (2017) and have reproduced their reported results. For the WMT14 dataset, the `base` Transformer is used, which consists of a 6-layer encoder and a 6-layer decoder. The size of the hidden units and embeddings is 512 and the number of heads is 8. The `big` Transformers has 1024 hidden units and 16 heads, which is listed as a reference. For IWSLT14 dataset, the `small` setting is used and the number of heads in every layer is set to 4. All the configurations are kept the same when applying our method or the regularization method. In our method, only the training process is changed and SVGD update rule is utilized in our algorithm. The stepsize ϵ in our method is set to 0.1 and the repulsive term α is set to 0.01. The Transformer-*small* model is trained on one TITAN Xp GPU. The Transformer-*base* model is trained on four GTX 1080Ti GPUs.

B.2.4 ELECTRA

Dataset Following the official code of Clark et al. (2020), ELECTRA models are pretrained on the OpenWebTextCorpus⁹ dataset, an open source effort to reproduce OpenAI’s WebText dataset. OpenWebTextCorpus contains 38GB of text data from 8,013,769 documents. The pretrained model is then finetuned and evaluated on GLUE benchmark¹⁰. GLUE contains a variety of tasks covering textual entailment (RTE and MNLI) question-answer entailment (QNLI), paraphrase (MRPC), question paraphrase (QQP), textual similarity (STS), sentiment (SST), and linguistic acceptability (CoLA). Our evaluation metrics are Spearman correlation for STS, Matthews correlation for CoLA, and accuracy for the other GLUE tasks.

Experiment settings The ELECTRA-*small* model we implemented follow all official settings¹¹ except that it is fully-trained on one GTX 1080Ti GPU for 6 days. The ELECTRA-*small* model has 12 layers with 4 heads in every layer’s attention. For our method, the stepsize ϵ is set to 0.01 and the repulsive term α is set to 0.1. The repulsive learning of attention is only applied to the pre-training stage. The fine-tuning remains the same with the original one.

B.2.5 GraphWriter

Dataset Experiments are conducted on the Abstract GENeration DAtaset (AGENDA) (Koncel-Kedziorski et al., 2019), a dataset of knowledge graphs paired with scientific abstracts. It consists of 40k paper titles and abstracts from the Semantic Scholar Corpus taken from the proceedings of 12 top AI conferences. We use the standard split of AGENDA dataset in our experiments: 38,720 for training, 1000 for validation, and 1000 for testing.

Experimental settings We follow the official settings¹² in Koncel-Kedziorski et al. (2019) with the encoder containing 6 layers and 4-head graph attention in every layer. We reproduce their results and keep all settings the same when applying the proposed repulsive attention. The SVGD update rule is used in our algorithm and applied to all layers. The stepsize ϵ is set to 0.1 and the repulsive weight is set to 0.01 in this experiment. The model is trained on one TITAN Xp GPU.

B.3 Computational Complexity

The main additive computational cost of repulsive attention training is caused by the pairwise kernel of the parameters of attention heads. Consider there are M heads in one attention module and the flattened dimension of every head is D_θ , then the time complexity is $O(M^2 D_\theta)$. For the regularization approach in Li et al. (2018), the time complexity is the same with us if the cosine similarity regularization is applied to attention parameters. But they find that the regularization of attention outputs $\{Z_i\}_{i=1}^M$ yielding the best performance. In this case, the time complexity is $O(BM^2 D_z)$ with the batch size B and the flattened hidden dimension D_z of latent representation Z_i , which leads to more training time with large batch size and long sentences.

⁸<https://github.com/pytorch/fairseq>

⁹<https://skylion007.github.io/OpenWebTextCorpus/>

¹⁰<https://gluebenchmark.com/>

¹¹<https://github.com/google-research/electra>

¹²<https://github.com/rikdz/GraphWriter>

C Additional Analysis of Our Approach

C.1 Comparison with SGLD

We also conducted a comparison of our method with Stochastic gradient Langevin dynamics (SGLD) ([Welling and Teh, 2011](#)), which is also a Bayesian sampling method. Results are in Table 8. Though random noise brought by SGLD might help achieving diversity, it's sub-optimal. Using particle-optimization to add the repulsive term makes it more effective.

Sampling Method	Age	Yelp	SNLI	IWSLT14 De-En
None	81.47	69.3	83.79	34.4
SGLD	81.57	70.1	83.80	34.7
SVGD	81.82	71.2	84.58	35.2

Table 8: Performance of attention models with different sampling methods on four tasks. For Age, Yelp and SNLI sentence classification tasks, the evaluation metric is accuracy (%). For IWSLT14 De-En translation task, the evaluation metric is BLEU score. "None" here means the standard multi-head attention models.

C.2 What Prior to Use?

In our approach, the repulsiveness is imposed by the inference algorithm (*i.e.* SVGD), not prior. To study the impact of different priors, we also tested the Gaussian prior. We found that (see Table 9) different priors have little impact on the final results, *i.e.*, there is not a consistent winner for different priors. This suggests that, the prior has little impact on repulsiveness in our framework. But one can still impose prior knowledge of the attention to help our algorithm learn a better attention model. We would like to explore that in future works.

Prior	Age	Yelp	SNLI
Uniform	81.82	71.7	84.58
Gaussian	81.88	71.6	84.28

Table 9: Performance of our approach with different priors on three sentence classification tasks. The evaluation metric is accuracy (%)

C.3 Which attention modules to be diversified?

Models	BLEU	Time
MA	34.4	1
RMA (Q)	34.7	1.06
RMA (K)	34.7	
RMA (V)	34.9	
RMA (En)	34.6	1.06
RMA (De)	34.7	
RMA (En-De)	34.9	
RMA (first layer)	35.1	1.03
RMA (last layer)	34.7	
RMA (All)	35.2	1.13

Table 10: Ablation study of Transformer-small-RMA model on IWSLT14 De-En dataset with repulsive multi-head attention applied on different part of the model. En: self-attention in encoder. De: self-attention in decoder. En-De: inter-attention between encoder and decoder. Time: relative training time of every step versus MA.

There are three types of attention in Transformer: self-attention in the encoder, self-attention in the decoder, and inter-attention between the encoder and decoder. We conduct extra experiments on Transformer-small to investigate which attention module benefits most from the repulsiveness. Results

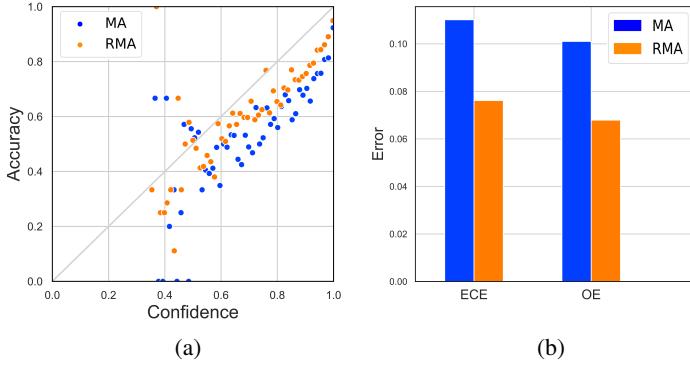


Figure 4: (a) Scatterplots for accuracy and confidence for SNLI test set. The repulsive case (RMA) is much better calibrated with the points lying closer to the $y = x$ line, while in the standard case (MA), points tend to lie in the overconfident region. (b) Expected Calibration Error (ECE) and Overconfidence Error (OE) for two cases.

are shown in Table 10. We first apply the repulsive attention on each of {Q,K,V} parameters in every attention module for all layers. The results indicate that diversifying the V-parameter seems to yield better performance. We then compare repulsive attention inside the encoder, inside the decoder and between them, respectively. The results show improvement in all cases, and diversifying inter-attention seems to achieve the most benefit. Finally, we diversify the attention in different layers of the Transformer. The results suggest that only diversifying the attention in the first layer is able to achieve comparable performance to the case of diversifying all layers, with little computational time increased.

C.4 Improved Calibration

A reliable model must not only be accurate, but also indicate when it is likely to get the wrong answer. It means the confidence of a well calibrated model should be indicative of the actual likelihood of correctness. Following the calibration metrics in Guo et al. (2017) and Thulasidasan et al. (2019), we evaluate the calibration of the model in Figure 4. For classifiers, the predicted softmax scores of winning class are represented as the confidence of models. Expected Calibration Error (ECE) and Overconfidence Error (OE) are two calibration metrics evaluating the reliability of a model. Following Guo et al. (2017) and Thulasidasan et al. (2019), softmax predictions are grouped into M interval bins of equal size. Let B_m be the set of samples whose prediction scores (the winning softmax score) fall into bin B_m . The accuracy and confidence of B_m are defined as

$$\text{acc}(B_m) = \frac{1}{|B_m|} \sum_{i \in B_m} \mathbf{1}(\hat{y}_i = y_i) \quad (10)$$

$$\text{conf}(B_m) = \frac{1}{|B_m|} \sum_{i \in B_m} \hat{p}_i \quad (11)$$

where \hat{p}_i is the confidence (winning score) of sample i . The Expected Calibration Error (ECE) is then defined as:

$$\text{ECE} = \sum_{m=1}^M \frac{|B_m|}{n} |\text{acc}(B_m) - \text{conf}(B_m)| \quad (12)$$

In high-risk applications, confident but wrong predictions can be especially harmful. Overconfidence Error (OE) is defined as follow for this case.

$$\text{OE} = \sum_{m=1}^M \frac{|B_m|}{n} [\text{conf}(B_m) \times \max(\text{conf}(B_m) - \text{acc}(B_m), 0)] \quad (13)$$

As shown in Figure 4, the standard attention model is prone to be over-confident, meaning that the accuracy is likely to be lower than what is indicated by the predictive score. With the proposed repulsive training of

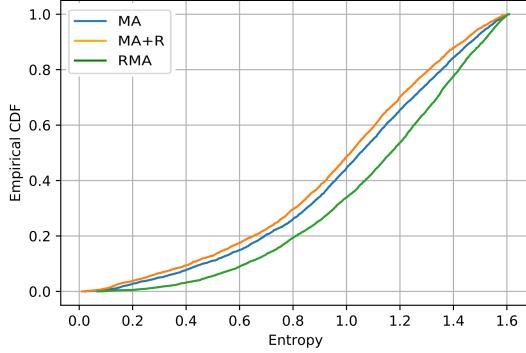


Figure 5: Empirical CDF for the entropy of the predictive distributions on Age dataset from the model trained on Yelp dataset. Curves that are closer to the bottom right part of the plot are preferable, as it denotes that the probability of observing a high confidence prediction is low.

Methods	Acc(%)	
	Age	Yelp
cosine similarity regularization	81.35	68.50
$i -> j$	81.65	71.45
$i -> j$, +smooth	81.85	71.50

Table 11: Adapt cosine similarity regularization on attention parameters gradually to our framework. Accuracy of the model is evaluated on the test set of Age and Yelp dataset.

attention, the model becomes better calibrated with much lower calibration error and overconfidence error, indicating that our method is beneficial for training more reliable multi-head attention models.

C.5 Improved Uncertainty Prediction

We follow Louizos and Welling (2017) to evaluate the predictive uncertainty. We estimate the entropy of the predictive distributions on Age dataset (out-of-distribution entropy) from the models trained on Yelp dataset. Since we a-priori know that none of the Age classes correspond to a trained class (they are two different tasks), the ideal predictive distribution is uniform over the Age dataset, i.e. a maximum entropy distribution. We plot the empirical CDF for the entropy in Figure 5. It shows that the uncertainty estimates from the repulsive multi-head attention model is better than the standard attention and the regularization approach.

C.6 Discussion with Existing Regularization-based Methods

Learning diverse attentions has been proposed in Lin et al. (2017) and Li et al. (2018), with different regularization techniques to enforce repulsiveness. In fact, we can show that existing methods are simplified versions of our framework, but with a potential mismatch between their algorithm and the underlying repulsiveness guarantee. To explain this, we follow Li et al. (2018) and apply cosine similarity regularizer to the attention parameter θ . When negative log-likelihood is used as the loss function and the prior of $\theta^{(i)}$ is assumed to be uniform, the update function ϕ becomes:

$$\phi(\theta_\ell^{(i)}) = -\nabla_{\theta_\ell^{(i)}} U(\theta_\ell^{(i)}) + \nabla_{\theta_\ell^{(i)}} \frac{1}{M} \sum_{j=1}^M \frac{\theta_\ell^{(i)} \theta_\ell^{(j)}}{\|\theta_\ell^{(i)}\| \|\theta_\ell^{(j)}\|}$$

One can consider the cosine similarity as a kernel function. Applying this new kernel function to our framework results in the following update:

$$\phi(\theta_\ell^{(i)}) = \frac{1}{M} \sum_{j=1}^M -\frac{\theta_\ell^{(i)} \theta_\ell^{(j)}}{\|\theta_\ell^{(i)}\| \|\theta_\ell^{(j)}\|} \nabla_{\theta_\ell^{(j)}} U(\theta_\ell^{(j)}) + \frac{1}{M} \sum_{j=1}^M \nabla_{\theta_\ell^{(j)}} \frac{\theta_\ell^{(i)} \theta_\ell^{(j)}}{\|\theta_\ell^{(i)}\| \|\theta_\ell^{(j)}\|} \quad (14)$$

It is clear that our method (14) reduces to the regularizing method when 1) removing the smoothing term $\frac{\theta_\ell^{(i)} \theta_\ell^{(j)}}{\|\theta_\ell^{(i)}\| \|\theta_\ell^{(j)}\|}$ for $j \neq i$; and 2) replacing the derivative $\nabla_{\theta_\ell^{(j)}}$ with $\nabla_{\theta_\ell^{(i)}}$ in the repulsive term. For this reason, we argue that the regularization method lacks of a formal guarantee on the repulsiveness.

To show this, we adapt the cosine similarity regularization on attention parameters gradually to our framework by 1) replacing the derivative $\nabla_{\theta_\ell^{(i)}}$ with $\nabla_{\theta_\ell^{(j)}}$ in the repulsive term; 2) adding the smoothing term $\kappa(\theta_\ell^{(j)}, \theta_\ell^{(i)})$. Table 11 shows that both the smoothing and the corrected gradient lead to performance improvement over the standard regularization methods.

D Visualization of Multi-head Attention in Sentence Classification Task

(a) detailed attentions of 30 heads

the food was amazing and worth the dip in the pocketbook . a downfall was the atmosphere felt like a cafeteria . service was passing .

(b) overall attention

Figure 6: Attention heatmaps for the standard multi-head attention model

(a) detailed attentions of 30 heads

the food was amazing and worth the dip in the pocketbook . a downfall was the atmosphere felt like a cafeteria . service was passing .

(b) overall attention

Figure 7: Attention heatmaps for the standard multi-head attention model trained with Frobenius regularization

(a) detailed attentions of 30 heads

the food was amazing and worth the dip in the pocketbook . a downfall was the atmosphere felt like a cafeteria . service was passing .

(b) overall attention

Figure 8: Attention heatmaps for the repulsive multi-head attention model

we order a fruits bag per week to be shared for in our small office . me likes that : - the produce is fresh - delivery is reliable and prompt - support is friendly and quick to respond - you get to customize your own weekly bag if you find there 's something you do n't like in it (or never want to receive again for whatever reason / allergies) - the delivery is made in a cooler bag with an ice pack inside , lovely for warm days me no likes that : - the vegetables are so fresh they 're positively unripened . seriously , our green bananas go rotten before they ever turn yellow - some of the fruits are imperfect (i 'm talking holes in apples , bruised fruit , black / mushy spots) - the fruits are never very sweet and tend to be on the sour to extremely sour side - a lot of times it seems that fruits go out of stock and you do n't find out until the delivery 's already been made - you 're credited the amount , but it would be nice to know in advance of the delivery so you can add other items to it if desired - no deliveries are made on mondays the produce is still way better than another organic grocer that we 've tried though , so we 'll be sticking with fresh city !

(a) example 1

my husband and i received a gift certificate for a night at the arbor house for our wedding , and we are so glad we did ! we were greeted by inn owner cathie , who immediately made us feel welcome as she showed us to our room . we stayed in the john nolen room , which is beautifully decorated , has a very comfy bed and boasts a 2-person hot tub (complete with great - smelling bubble bath to enjoy a fully relaxing soak !) . we enjoyed some refreshing margaritas in the lobby before heading out to dinner (there are some excellent restaurants nearby) . upon returning , we gobbled down our sweet treat that the inn offers nightly - scrumptious ! what impressed me most during our stay was how cathie adapted the morning breakfast to fit my dietary allergies , which i mentioned to her the night before . when i brought it up , she immediately began going through her planned menu and figured out how she would adjust the dishes to make them ok for me to eat . i was touched by this extra effort - and the breakfast was absolutely delicious ! our stay was completely enjoyable and relaxing , and we recommend the arbor house wholeheartedly !

(b) example 2

this review is strictly for the las vegas suites property management company and not the mgm signature suites hotel . las vegas suites manages certain rooms in this hotel and we had the misfortune of staying in one of them on our recent trip to vegas . staying in a room managed by lvs is a much different experience than staying in a room that 's actually part of the mgm hotel . the reason we booked this stay to begin with was because we had stayed here previously and had a great experience , but we stayed in an mgm managed suite . this time , i booked the room through expedia and did n't pay attention the small print when i paid for the room (does anyone really look at that stuff ?) big mistake on my part . upon checking into the hotel we immediately noticed a few things that were instantly different from our last stay . first of all , when i made the room reservation , i specifically stated through expedia that we wanted a room on a high floor away from the elevators . my wife and i are very sensitive to noise and , having travelled extensively , know that rooms near the elevators tend to be the noisiest so we wanted to be as far away as we could . the front desk person told us that not only had they booked us right next to the elevator , but we were overlooking the pool which has a dance party every day from 11 am - 5 pm . she did n't think it would be a big deal though as the room was still not very close to the elevator doors and you could n't hear the music from the party with the balcony doors closed . we asked to switch our room , but she said since we had booked through lvs we had to contact them and they would n't be open until tomorrow . when we got into the room we instantly saw several things amiss : 1) the room features a guest bathroom with a shower stall which my kids were going to use since they were sleeping in the living room . the floor of the shower was filthy with black dirt particles left over from who knows how long ago (see picture) 2) the sofa bed mattress that my kids were going to be sleeping on had huge holes and gashes on the bottom that looked like rats had been gnawing on (see picture) 3) the wireless phone in the living room did n't work at all 4) there were stains on the living room carpet underneath the coffee table (see picture) 5) furniture in the unit had holes or visible signs of wear (see picture) 6) the outside balcony was filthy and looked like the glass had not been cleaned in some time (see picture) 7) not only did they put us in a room that was overlooking the pool party , but we were directly adjacent to a construction site that started work every morning at 6 am (see picture and video) now , i understand that hotels ca n't predict when construction is going to be going on next to their property , but you would think that someone scheduling the rooms would look at our request and think , hmm these people do n't want to be near the elevator - they probably would like a room in the quiet part of the hotel . i seriously do n't think anyone actually looks at those special room requests anyway so it was probably just wishful thinking on my part . there was also a sign in the room that was essentially a menu for cleaning services . if we want to have the room cleaned on a daily basis it would be \$ 50 , if we wanted clean towels it would \$ 20 - yes , that 's right \$ 20 for clean towels . i considered us lucky that they granted us an extra roll of toilet paper in our unit . who knows how much extra that would have cost ? i did see in the small print on our itinerary that there would be a \$ 50 cleaning fee based on the size of the unit , but again , i 've never stayed in a hotel that charged for cleaning so i did n't pay any attention to it . i guess that 's the last time i skip the fine print . when i tried to call lvs the next day i spoke to a fairly rude woman on the phone who told me that she was sorry , but they were fully committed and could n't move our room and since no special requests had been made for a quiet room they could n't make any concessions for us . i asked if her if there was anything they could do as far as maybe giving us a discount or a food and beverage credit and she flat out refused . basically , what we learned is that when you stay in a suite that 's managed by lvs you are completely on your own . we even tried calling down to the front desk for a pair of scissors one night and were told that since we were not hotel guests they could n't provide us with one . if you are looking to stay at the signature suites do yourself a favor and book directly through the hotel . las vegas suites is a sorry excuse for a company that only cares about their bottom line and could n't give a rats ass what their customers think . oh , and annabelle r . , do n't bother writing a snarky response to my review as you have done with everyone else . it just makes you and your company look guilty and desperate to cover up your faults rather than trying to appease an extremely unsatisfied customer .

(c) example 3

Figure 9: Overall attention heatmaps of Yelp reviews with standard multi-head attention

we order a fruits bag per week to be shared for in our small office . me likes that : - the produce is fresh - delivery is reliable and prompt - support is friendly and quick to respond - you get to customize your own weekly bag if you find there 's something you do n't like in it (or never want to receive again for whatever reason / allergies) - the delivery is made in a cooler bag with an ice pack inside , lovely for warm days me no likes that : - the vegetables are so fresh they 're positively unripened . seriously , our green bananas go rotten before they ever turn yellow - some of the fruits are imperfect (i 'm talking holes in apples , bruised fruit , black / mushy spots) - the fruits are never very sweet and tend to be on the sour to extremely sour side - a lot of times it seems that fruits go out of stock and you do n't find out until the delivery 's already been made - you 're credited the amount , but it would be nice to know in advance of the delivery so you can add other items to it if desired - no deliveries are made on mondays the produce is still way better than another organic grocer that we 've tried though , so we 'll be sticking with fresh city !

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(c) example 3

Figure 10: Overall attention heatmaps of Yelp reviews with repulsive multi-head attention

E A Generation Sample of Graph-to-Text Task

Title	Bilinear signal synthesis in array processing
Knowledge	(source positions, CONJUNCTION, angular separations); (time-frequency synthesis techniques, USED-FOR, multiple source signals); (non-integer values, USED-FOR, weighing function); (weighing function, USED-FOR, time-frequency domain); (quadratic t-f distributions, USED-FOR, source separation techniques); (spatial time-frequency distributions, USED-FOR, blind source separation methods); (time-frequency synthesis techniques, USED-FOR, antenna array)
GraphWriter	In this paper, we propose a novel method for blind source separation methods based on a weighing function. In the proposed method, the spatial signatures of sources is modeled as a weighing function, and the spatial time-frequency distributions is modeled as a weighing function. The spatial time-frequency distributions is modeled as a weighing function in the time-frequency domain. The proposed method is based on the use of a weighing function to estimate the parameters of the blind source separation methods. The proposed method is based on the use of a weighing function to estimate the parameters of the blind source separation methods. The proposed method is applied to the problem of multiple source signals in the time-frequency domain. The proposed method is applied to the problem of multiple source signals in the time-frequency domain. The proposed method is shown to be robust to noise levels, whitening, and angular separations.
+ RMA	In this paper, we present a novel approach to multiple source signals based on the spatial signatures of sources and angular separations. In particular, we consider the problem of estimating the spatial signatures of sources from a single image of an antenna array. We propose a novel method for estimating the spatial signatures of sources using a weighing function, where the source positions and angular separations are estimated in a time-frequency domain. We show that the proposed method can be used to derive a weighing function for the communication channel. The proposed method is based on the use of quadratic t-f distributions in the time-frequency domain and the non-integer values. The proposed method is applied to the problem of whitening and angular separations. The experimental results show that the proposed method is more robust to noise levels and noise levels.
Gold	Multiple source signals impinging on an antenna array can be separated by time-frequency synthesis techniques. Averaging of the time-frequency distributions of the data across the array permits the spatial signatures of sources to play a fundamental role in improving the synthesis performance. Array averaging introduces a weighing function in the time-frequency domain that decreases the noise levels, reduces the interactions of the source signals, and mitigates the crossterms. This is achieved independent of the temporal characteristics of the source signals and without causing any smearing of the signal terms. The weighing function may take non-integer values, which are determined by the communication channel, the source positions and their angular separations. Unlike the recently devised blind source separation methods using spatial time-frequency distributions, the proposed method does not require whitening or retrieval of the source directional matrix. The paper evaluates the proposed method in terms of performance and computations relative to the existing source separation techniques based on quadratic t-f distributions.

Figure 11: Example outputs of various systems versus Gold