Implicit Kernel Attention

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Abstract

Attention compute the dependency between representations, and it encourages the model to focus on the important selective features. Among the attention methods, the scaled dot-product attention is widely utilized in many models. This paper suggests a generalized structure of the scaled dot-product attention with similarity and magnitude terms. We derive that the scaled dot-product attention is a product of two parts: 1) the RBF kernel to measure the similarity of two instances and 2) the exponential $L^2$ norm to compute the importance of individual instances. From this decomposition, we improve the attention in two ways: implicit modeling on the kernel spectral density and generalized $L^p$ norm, which results in a learnable and flexible attention structure. First, we estimate the spectral density of kernel with implicit probabilistic models to estimate the appropriate kernel for a given dataset without kernel selection manually. Second, we introduce a generalized $L^p$ norm on the hidden feature space, where $p$ is a hyper-parameter that affects the scale of individual importance and the sparsity of attention weights. Also, we show how to expand this implicit kernel modeling to multi-head attention in conjunction with a copula augmentation. Our generalized attention shows better performance on text classification, translation, regression, and node classification tasks.

1 Introduction

In neural networks, Attention has become an essential structure. Attention captures the important features and allows the model to focus on the essential features. The attention method is crucial in improving the model performance as well as explaining the model mechanisms, and many models utilize the scaled dot-product attentions. The scaled dot-product attention compute the dot-product between query and key, which is a linear projection of hidden feature. It is well known that the dot-product of two vectors is a product of two terms, 1) cosine of the angle between two vectors, which denotes the similarity, 2) norm of each vector which measures individual scale. In this paper, we further analyze the meaning of scaled dot-product attention. Because the scaled dot-product attention uses an un-normalized dot-product between query and key, the attention weights are influenced by 1) similarity between query and key, relative importance, and 2) the magnitude of each query and key, individual importance. This opens a question on how to separate the scaled dot-product attention as the similarity and magnitude term explicitly, which have different meanings, and how to generalize it.

This paper formalizes generalized scaled dot-product attention by translating the attention weight into a multiplication of two terms: similarity and magnitude. We derive the explicit separation in Proposition[1] that the scaled dot-product attention is a product of 1) the Radial Basis Function (RBF) kernel function between query and key with fixed hyper-parameters, and 2) exponential of $L^2$ norm for each representation vectors.

After the formalization of attention with similarity and magnitude, the kernel function measures the similarity under the inductive bias of each kernel. The measurement can be further flexible by
adopting an implicit kernel function, instead of kernel manual selection. This bias often calls upon a modeler’s manual kernel selection by domains and datasets. Hence, we generalize this explicit kernel function, embedded in the scaled dot-product attention, by an implicit kernel function. In particular, the kernel is isomorphic to its double dual so that the kernel estimation problem can be interpreted as the spectral density estimation [1][2]. We formulate the implicit kernel function by estimating the spectral density depending on the dataset. This generalization interprets kernel learning as the spectral density estimation [3,4], and it can be further elaborated by structured modeling i.e. Gaussian copula.

The second component of scaled dot-product attention is the magnitude term, which measures the importance of each query and key by an exponential of $L^2$ norm. As $L^2$ norm in the scaled dot-product attention is rigid without considering the dataset property, we can extend it to be a $L^p$ norm with a hyper-parameter $p$. The hyper-parameter $p$ controls the growth rate of the magnitude terms, and this growth is eventually related to the sparsity of the attention weights.

The combination of generalized implicit kernel function and generalized $L^p$ norm results in a more flexible attention structure. The new attention structure is exchangeable with the attention in Transformer, GAT, etc. Our attention methods provide an improvement in performance on classification, translation, and regression tasks.

2 Preliminary

2.1 Attention

In neural networks, attention compute the alignment matrix between feature representations and encourage the model to focus on the important selective representations. While the alignment can be measured in diverse ways, the scaled dot-product attention calculates the importance weight by the dot-product of $q_i = h_iW_Q$ and $k_j = h_jW_K$ with the hidden feature $h$; the query $q_i$; the key $k_j$; and linear projection matrix $W_Q, W_K$ [5]. The scaled dot-product attention weight $\alpha_{ij}$ in Eq. [1] is the output from the softmax function of the dot-product on $q_i$ and $k_j$ with a scaling, $1/\sqrt{d_k}$, where $d_k$ is the dimension of $k_j$.

$$\alpha_{ij} = \frac{\exp(q_i^Tk_j^T/\sqrt{d_k})}{\sum_i \exp(q_i^Tk_j^T/\sqrt{d_k})}$$ \hspace{1cm} (1)

There are many neural network models with attention, such as Transformer [5] and Graph attention network (GAT) [6]. Transformer utilizes the scaled dot-product to compute the attention weights, and its extended version, Multi-Head scaled Attention (MHA), by introducing the attention head index $m$ in $W_Q^{(m)}$ and $W_K^{(m)}$. Graph attention network (GAT) [6] also adopts the attention structure to aggregate the relevant neighborhood’s features in the message passing phase. GAT calculates the weight as $\alpha_{ij} = \exp(g(h_i, h_j))/\sum_{j \in N_i} \exp(g(h_i, h_j))$ for neighbor of a node $i$, $N_i$, and $g$ can be the scaled dot-product while other choices are feasible, as well.

2.2 Kernel

Spectral density Kernel is a self-dual under the Fourier transformation [7], and stationary continuous kernel approximation becomes the estimation of the spectral density $p(w)$ in Eq. [2] with $R$ sampled spectral points $w_r$.

$$K(x - x') = \int_{RD} \exp(iw^T(x - x')) dp(w) \approx \frac{1}{R} \sum_{r=1}^{R} \exp(iw_r^T(x - x'))$$ \hspace{1cm} (2)

We can represent a stationary continuous kernel with the expectation of the spectral density under the Bochner’s theorem [1]. Similar to the stationary kernel, the Yaglom Theorem ensures the existence of the Fourier dual of the positive definite non-stationary continuous kernel [2]. Under the Bochner theorem, Li et al. [3] learn kernel function by estimating the spectral density with an implicit generative model, a generator in Generative Adversarial network [8].

\footnote{We provide a further empirical analysis of the kernel on word embedding in Appendix C.}

\footnote{We provide empirical analysis between $L^p$ norm and sparsity of attention weights in Appendix C.}
We interpret that the scaled dot-product has two components, the similarity, and the magnitude. The scaled dot-product has the similarity term, \( f_{\text{sim}}(\mathbf{q}_i, \mathbf{k}_j) = \exp(-\|\mathbf{q}_i - \mathbf{k}_j\|^2 / 2\sqrt{d_k}) \), which is the RBF kernel with fixed length-scale hyper-parameters, \( \sqrt{d_k} \), which determines the smoothness. Additionally, the scaled dot-product yields the magnitude term, \( f_{\text{mag}}(\mathbf{q}_i, \mathbf{k}_j) = \exp(-\|\mathbf{q}_i\|^2 / 2\sqrt{d_k}) \times \exp(-\|\mathbf{k}_j\|^2 / 2\sqrt{d_k}) \), and it measures the individual importance of each instance as \( \|\mathbf{q}_i\|_2^2 \) and \( \|\mathbf{k}_j\|_2^2 \) with \( L^2 \) norm. From the factorization, we propose a new attention method which formulates an implicit kernel function and utilizes a generalized \( L^p \) norm.

### 2.3 Copula

As MHA introduces the multiple vectors of attention weights, these weights are expected to capture the diverse aspects of representation. The MHA lacks explicit modeling to handle the dependency between multiple attentions. Transformer expects its MHA to capture different aspects by randomly initializing the linear projection matrix in each head. We formulate a copula-augmented spectral density estimation to consider the dependency between the spectral densities in each head. The copula is a cumulative distribution function (CDF) defined on the unit cube with uniform univariate marginals \([0,1]\). Formally, copula \( C \) is defined as \( C(u_1, \ldots, u_d) = P(U_1 \leq u_1, \ldots, U_d \leq u_d) \), where marginal on \( U_i \) is uniformly defined on \([0,1]\). By Sklar’s theorem \([11]\), we can represent a joint cumulative distribution of \( x_1, \ldots, x_d \) as a marginal distribution of each random variables and their copula, \( F(x_1, \ldots, x_d) = C[F_1(x_1), \ldots, F_d(x_d)] \). We impose the dependencies between attentions in MHA by estimating each head’s spectral density jointly with copula augmented inference.

### 3 Methodology

We interpret that the scaled dot-product has two components, the similarity, and the magnitude. The similarity measures the relative importance and magnitude to compute individual importance. To analyze the role of two components that have different meanings, and generalize them, we decompose the scaled dot-product attention into two distinct exponential terms: 1) the similarity term and 2) the magnitude term in Proposition\(^3\).

**Proposition 1.** Let \( \alpha_{ij} \) be an attention weight given by Eq. \( \text{(1)} \). Then \( \alpha_{ij} \) has the form:

\[
\alpha_{ij} = \exp\left(-\frac{||q_i - k_j||^2}{2\sqrt{d_k}}\right) \times \exp\left(-\frac{||q_i||^2 + ||k_j||^2}{2\sqrt{d_k}}\right) / \sum_{l}(\exp\left(-\frac{||q_i - k_l||^2}{2\sqrt{d_k}}\right) \times \exp\left(-\frac{||q_i||^2 + ||k_l||^2}{2\sqrt{d_k}}\right))
\]

The scaled dot-product has the similarity term, \( f_{RBF} = \exp(-\|q_i - k_j\|^2 / 2\sqrt{d_k}) \), which is the RBF kernel with fixed length-scale hyper-parameters, \( \sqrt{d_k} \), which determines the smoothness. Additionally, the scaled dot-product yields the magnitude term, \( \exp(-\|q_i\|^2 / 2\sqrt{d_k}) \times \exp(-\|k_j\|^2 / 2\sqrt{d_k}) \), and it measures the individual importance of each instance as \( \|q_i\|_2^2 \) and \( \|k_j\|_2^2 \) with \( L^2 \) norm. From the factorization, we propose a new attention method which formulates an implicit kernel function and utilizes a generalized \( L^p \) norm. First, we propose implicit kernel attention (IKA), and IKA learns an appropriate kernel.

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\(^3\)The proof is given in Appendix D.
shape and its hyper-parameters by a data-driven approach. Second, we interpret $p$ in $L^p$ norm as a hyper-parameter, so we define IKA with norm (IKAN), which improves IKA by changing $L^p$ norm to control the magnitude of independent importance and the sparsity of attention weights. Third, we propose multi-head IKAN (MIKAN), which adopts a copula-augmented inference to estimate a structured spectral density of MHAs jointly.

The scaled dot-product attention uses a fixed Gaussian spectral density $p(w)$ and a RBF kernel in Figure 1a. In contrast, IKA, IKAN, and MIKAN estimates the spectral density to find an appropriate kernel depending on the dataset. As an alternative of IKA and IKAN in Figure 1b, we propose a deterministic model, IKAN-direct, that optimize spectral points $w$ directly in 1c. MIKAN estimates the joint spectral density in Figure 1d, while the IKA and IKAN estimate the spectral density individually for each head of attention. Figure 1c represents the structure overview of our models.

### 3.1 IKA: Implicit Kernel Attention

The scaled dot-product attention depends on the RBF kernel, and the RBF measures the similarity by the Euclidean distance. Since a deep network embeds the data manifold into the hidden feature space through the combination of the linear transformations and the non-linear activation functions, the Euclidean metric may not be proper in modeling the hidden space. Furthermore, the RBF includes the exponential term, and it prevents the attention from representing the sparse attention weights.

Because the kernel is a self-dual under the Fourier transformation [1][2], we can approximate kernel with the spectral density $p(w)$. The flexible spectral density estimation allows us to construct implicit kernel, while the spectral density of the RBF kernel is a zero-mean Gaussian distribution. An implicit probabilistic model is necessary to estimate the spectral density flexibly instead of a fixed distribution form. We can formulate an implicit probabilistic model in two steps. The first step constructs a base distribution, $p(z)$, such as a Gaussian distribution, and we sample $z$ from $p(z)$. The second step transforms the sampled $z$ with a flexible function such as a neural network to estimate the spectral density $p(w)$. It is noted that both the base distribution and the spectra density should be symmetric.

Under the implicit probabilistic model, the log marginal likelihood, $\log p(y|h)$, is intractable where $y$ is a output variable and $h$ is a hidden feature. Therefore, we derive the evidence lower bound (ELBO) [12] of the log marginal likelihood with inference network, $q(z|h)$. We maximize the ELBO in Eq. [3] with re-parameterization method to backpropagate the gradients [12].

$$L = E_{q(z|h)}[\log p(y,z|h)] - E_{q(z|h)}[\log q(z|h)]$$  \hspace{1cm} (3)

For MHAs in Transformer or GAT, we sample $z$ from a $q(z|h)$ for each head independently, by formulating $q(z|h) = \prod_{m=1}^{M} q(z^{(m)}|h^{(m)})$. We construct each inference network $q(z^{(m)}|h^{(m)})$ with neural network parameterized by $\psi_1$ as in Eq. 4. We formulate $z^{(m)}$ as a concatenation of $z^{+(m)}$ and $z^{-(m)}$ to preserve the symmetric of a base distribution.

$$\mu^{(m)}, \log \sigma^{(m)} = NN_{\psi_1}(h^{(m)}), \quad z^{+(m)} \sim N(\mu^{(m)}, (\sigma^{(m)})^2), \quad z^{-(m)} \sim N(-\mu^{(m)}, (\sigma^{(m)})^2)$$  \hspace{1cm} (4)

With symmetric base distribution, we can use any function to estimate the spectral density by preserving symmetric property with simple additional treatment. After sampling $z^{(m)}$, we follow the second step, transforming $z^{(m)}$ with neural network $NN_{\psi_2}$ to estimate the spectral density flexibly in Eq. 5. To preserve the symmetric property of the spectral density, we use the absolute value of $|z^{(m)}|$ as an input, and we multiply the sign of $z^{(m)}$ in Eq. 5.

$$w^{(m)} = \text{sign}(z^{(m)}) \times NN_{\psi_2}(|z^{(m)}|)$$  \hspace{1cm} (5)

With implicit probabilistic model, we can sample spectral points $w$ flexibly, and we calculate the implicit kernel function $f$ and attention weights $\alpha_{ij}$ in Eq. 6. The implicit kernel function is a similarity term of attention in Proposition 1. The rest of structure is same with Transformer with neural network $NN_{\psi_3}$ in Eq. 7.

$$\alpha_{ij}^{(m)} = \frac{\tilde{\alpha}_{ij}^{(m)}}{\sum_l \tilde{\alpha}_{il}^{(m)}} \quad \text{where} \quad \tilde{\alpha}_{ij}^{(m)} = f(q_i^{(m)}, k_j^{(m)}, w^{(m)}) \times \exp\left(\frac{\|q_i^{(m)}\|^2 + \|k_j^{(m)}\|^2}{2\sqrt{d_k}}\right)$$  \hspace{1cm} (6)

$$\tilde{y} = NN_{\psi_3}(\alpha^{(1:M)}, h^{(1:M)})$$  \hspace{1cm} (7)
Because we do not assume any explicit distribution for \( w^{(m)} \), our model can approximate any continuous kernel, including RBF by the implicit probabilistic model and \( z^{(m)} \). This structure fundamentally depends upon the random Fourier features, so the next section explains the kernel construction with such features. For simplicity, we omit multi-head related notation \( m \).

IKA(S): Implicit Kernel Attention with Stationary kernel

We can approximate any continuous stationary kernel with the Monte Carlo (MC) integration with \( R \) sampled spectral points and its random Fourier feature map, \( \phi \), by taking the real part \([4, 13]\).

\[
\begin{align*}
  f(q_i, k_j, w) &= \frac{1}{R} \sum_{r=1}^{R} \phi_r(q_i) \phi_r(k_j) \\
  \phi_r(q_i) &= \left( \cos(w^T_1 q_i), \sin(w^T_1 q_i) \right), \quad \phi_r(k_j) = \left( \cos(w^T_2 k_j), \sin(w^T_2 k_j) \right)
\end{align*}
\]

(8)

We generalize the scaled dot-product attention by replacing the RBF in the scaled dot-product attention with \( f \). We name this attention as IKA(S). Since the output of the kernel function in Eq. 8 might have a negative value from its construction, we square Eq. (8), \( f^2 \), to assure the positiveness. Proposition 2 claims that the squared implicit kernel function still generalizes the RBF kernel.

**Proposition 2.** Let \( f \) be the RBF kernel function with lengthscale \( l \), and \( \hat{f} \) be its approximation with \( R \) random Fourier features by Eq. [8] and [9]. If we sample spectral points \( w \) from a Gaussian distribution \( N(0, \frac{1}{\sqrt{2\pi}}) \), then \( \lim_{R \to \infty} f^2 = f \).

IKA(NS): Implicit Kernel Attention with Non-Stationary kernel

Similar to the stationary kernel case, we can approximate any continuous non-stationary kernel with the random Fourier feature map \( \phi \) in Eq. [11] while we preserve the symmetric property \([4, 2]\).

\[
\begin{align*}
  f(q_i, k_j, w) &= \frac{1}{4R} \sum_{r=1}^{R} \phi_r(q_i) \phi_r(k_j) \\
  \phi_r(q_i) &= \left( \cos(w^T_1 q_i) + \cos(w^T_2 q_i), \sin(w^T_1 q_i) + \sin(w^T_2 q_i) \right), \quad \phi_r(k_j) = \left( \cos(w^T_1 k_j) + \cos(w^T_2 k_j), \sin(w^T_1 k_j) + \sin(w^T_2 k_j) \right)
\end{align*}
\]

(10)

(11)

Similar to IKA(S), we use \( f^2 \) instead of \( f \) to ensure the positiveness of the attention weight. We formulate new attention, IKA(NS), induced by non-stationary kernel function in Eq. [10][11]

3.2 IKAN: Implicit Kernel Attention with generalized \( L^p \) Norm

IKAN

In addition to the implicit kernel in IKA(NS), we generalize the \( L^2 \) norm in the scaled dot-product attention to be the \( L^p \) norm, which determines the individual representation importance and the sparsity of attention weights, as shown in Proposition 1. We show that attention weights become sparse when \( p \) goes to zero theoretically in Proposition 3. The optimal \( L^p \) norm might be different for each dataset and task, so we select \( p \) through experiments. Given that \( p \) influences on the sparsity, it plays a similar role as the temperature parameter, \( \tau \), in the Gumbel-softmax function \([14]\). However, these two parameters are different in two folds. First, \( p \) only affects the magnitude terms of each representation vectors without an association to the similarity term of the kernel, but \( \tau \) is associated with the entire logit calculation. Second, we prove that the adjusting weights sparse faster than adjusting \( \tau \) in Proposition 3.

**Proposition 3.** Let \( \alpha_{ij}(p, \tau) \) be \( \exp\left(\frac{-\|q_i - k_j\|^2}{2\tau^2d_n}\right) \times \exp\left(\frac{-\|q_i + k_j\|^2}{2\tau^2d_n}\right)/\sum_u \exp\left(\frac{-\|u - k\|^2}{2\tau^2d_n}\right) \times \exp\left(\frac{-\|u + k\|^2}{2\tau^2d_n}\right) \), \( A_{p, \tau} = \{1, \ldots, L\} \) and \( \alpha_{ij}(p, \tau) \) be a multi-dimensional indicator function, whose \( n \)-th component is 1 if \( n \in A_{p, \tau} \) and 0 otherwise.

i) \( \lim_{\tau \to 0} \alpha_{ij}(p = 2, \tau) = 1_{A_{p=2, \tau}}/A_{p=2, \tau} \)

ii) \( \lim_{\tau \to 0^+} \alpha_{ij}(p, \tau = 1) = 1_{A_{p=1, \tau=1}}/A_{p=1, \tau=1} \).

iii) Let \( f(t) = \alpha_{ij}(p = 2, \tau = t) \), \( g(t) = \alpha_{ij}(p = 2, \tau = 1) \) for \( i_1 \notin A_{p=2, \tau} \) and \( i_2 \notin A_{p, \tau=1} \).

Then, \( \lim_{\tau \to 0^+} \frac{g(t)}{f(t)} = 0 \)

\[4\] We define \( ||x||_p \) as \( (|x_1|^p + |x_2|^p + \ldots + |x_n|^p)^{1/p} \) for \( 0 < p \). \( ||x||_p \) defines a norm for \( 1 \leq p \), while \( ||x||_p \) defines an absolutely homogeneous function for \( 0 < p < 1 \).
**IKAN-direct**  We propose a simple but effective alternative model that sets spectral points $w$ as a learnable parameter such as a weight in a neural network. IKAN estimates the spectral density with a base distribution and implicit probabilistic model. Meanwhile, IKAN-direct optimizes $w$ directly.

### 3.3 MIKAN: Multi-Head Attention with IKAN

The dependency modeling between heads in MHA is necessary to diversify the attention weights. Similar to the individual calculation of the scaled dot-product attention in multiple heads, the variations of IKA estimate the spectral density in each head individually, and it can reduce the effectiveness of MHA. Therefore, we introduce $q(\mathbf{z}|h) = c_q(F_1(\mathbf{z}^{(1)}), \ldots, F_M(\mathbf{z}^{(M)})) \prod_{m=1}^{M} q(z^{(m)}|h^{(m)})$, where $c_q$ is a copula density; $F_m$ is a CDF of each $z^{(m)}$. This alternative variational distribution of $\mathbf{z}$ develops IKA to Multi-head IKAN (MIKAN) by introducing the joint structure through $c_q$. MIKAN maximizes ELBO in Eq. 5 with Monte Carlo estimation by sampling from $q(\mathbf{z}|h)$ \cite{12}. MIKAN alleviates the mean-field assumption by introducing copula-augmented posterior, and the IKAN is a special case of MIKAN if we fix $c_q$ as a uniform distribution \cite{15}. $c_q$ can be any copula density, and we set $c_q$ as a Gaussian copula with covariance, $\Sigma$.

### 4 Results

MIKAN is a generalized model of IKA(S), IKA(NS), IKAN, while IKAN-direct is a deterministic model that optimizes spectral points $w$ directly. We replace the existing attention structure with MIKAN or IKAN-direct in Transformer and GAT to compare the performance on the classification, translation, and regression tasks \cite{6}. We also include an ablation study for our models in Section 4.1.

#### 4.1 Sentence Classification

We compare our models with Transformer \cite{5}, RBF-only \cite{9}, Expsin, and Linear on six popular dataset \cite{16,17}. RBF-only represents the scaled dot-product attention with RBF kernel without magnitude term, and Expsin and Linear denote the scaled dot-product attention that uses periodic kernel and linear kernel with $L^2$ norm, respectively.

Table 1 represents that the appropriate kernel is different for each dataset. The Expsin performs better than other baselines on CR, MPQA, while Linear is better on SST. IKAN-direct and MIKAN that adopt implicit kernel function performs better than baselines consistently.

| Method    | CR       | MPQA     | MR       | SST      | SUBJ     | TREC     |
|-----------|----------|----------|----------|----------|----------|----------|
| Transformer | 77.4±1.8% | 82.1±1.0% | 71.1±1.0% | 71.4±2.7% | 88.4±0.6% | 72.9±3.0% |
| RBF-only  | 77.1±1.8% | 81.9±1.2% | 70.7±1.5% | 71.3±2.2% | 88.5±1.0% | 73.4±4.4% |
| Expsin    | 78.4±2.3% | 82.7±1.1% | 69.8±1.7% | 71.5±1.4% | 87.3±1.1% | 71.4±3.2% |
| Linear    | 78.2±2.6% | 82.1±1.2% | 69.2±1.9% | 71.9±2.0% | 87.5±0.8% | 70.9±3.8% |
| IKAN-direct | 79.1±2.1% | 82.9±0.9% | 73.7±0.8% | 75.5±0.8% | 89.3±0.7% | 82.8±1.1% |
| MIKAN     | 79.8±2.0% | 82.6±1.2% | 74.0±0.5% | 76.0±1.4% | 89.1±0.8% | 83.6±1.2% |

Table 1: Accuracy for the text classification task. The appropriate manual kernel selection is different for each dataset, but our model shows better performance consistently than other baselines.

Figure 2a shows the ablation study for our models. We can see the performance gain as the generalization level and capacity of models increases. Figure 2b,2c show attention weights for a given sentence on TREC. TREC requires classifying the question type of a sentence. The question type of the given sentence is numeric, and MIKAN focuses on "are worth what" in Figure 2b. Figure 2c shows the attention weights matrix for each head in IKAN, IKAN-direct, and MIKAN. MIKAN represents diverse attention weights across attention heads relatively.

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\[^{5}\text{We provide the detail explanation of MIKAN in Appendix A.}\]

\[^{6}\text{We provide results of the interpolation task for synthetic datasets in Appendix C.}\]

\[^{7}\text{We provide the detail experiment settings in Appendix B.}\]
Figure 2: (a): Ablation study for our models on the TREC dataset. (b): Average attention weights for the given sentence on TREC. TREC requires classifying the question type of a sentence. The question type of the given sentence is numeric, and our model MIKAN captures the "are worth what". (c): Attention weights matrix of each head for the given sentence. MIKAN capture the relatively diverse attention weights across the multi-head.

4.2 Translation

We compare the performance on the IWSLT14 De-En dataset, and we implement Transformer and our models with fairseq [18]. Table 2 shows that our models perform better than other models. We plot the similarity and the magnitude term in Transformer and our models to analyze the attention methods. Figure 3 represents the change in maximum similarity term and average magnitude term from the first epoch (start) to the last epoch (end). We set the last epoch for each model by the early stopping. We visualize the changes in the decoder-encoder cross attention layer (cross.), where pair-wise dependency is important for alignment between the source sentence and the target sentence. Figure 3 shows that the scaled dot-product attention in Transformer heavily depends on the magnitude term instead of similarity. The magnitude term in Transformer is relatively large even in an initial training step, and the value becomes greater in the last epoch. On the other hand, IKAN and MIKAN represent the relatively stable scale of similarity and magnitude term because of the generalized flexible implicit kernel and generalized $L_p$ norm. We see a similar tendency on the self-attention layer in Appendix C.

| Method                   | BLEU  |
|--------------------------|-------|
| Beam Search Optimization | 26.36 |
| Actor-Critic             | 28.53 |
| Neural PBMT + LM         | 30.08 |
| Minimum Risk Training    | 32.84 |
| Variational Attention    | 33.69 |
| Transformer              | 34.51 |
| IKAN-direct              | 34.81 |
| MIKAN                    | 34.57 |

Table 2: BLEU for IWSLT14 De-En.

Figure 3: Similarity and magnitude of decoder-encoder cross attention layer on IWSLT14 DE-En. Transformer heavily depends on the magnitude term, while our models show relatively stable similarity and magnitude term over the epoch.

4.3 Regression

Regression is an important problem, and it can be applied to many domains such as climate, real estate, and clinic. We apply Transformer on the UCI regression dataset and replace the scaled dot-product attention with our models. We perform 10-fold cross-validation and report the performance following [23]. Table 3 shows that our models perform better than other baselines. On the UCI regression dataset, we perform the qualitative analysis to clarify the relationship between $L_p$ norm and sparsity of attention weights empirically. Figure 4(a)-(c) visualize a histogram of MIKAN attention weights for different $p$ on Housing dataset. As $p$ goes to zero, most attention weights have either zero or one. Figure 4(d) shows the sensitivity analysis with respect to $p$. The RMSE varies depending on $p$, but all results show better performance than the baseline.
### Table 3: RMSE on the UCI Regression dataset.

| Method         | CO2    | Passenger | Housing | Concrete | Parkinsons |
|----------------|--------|-----------|---------|----------|------------|
| Transformer    | 0.057 ± 0.002 | 0.153 ± 0.043 | 0.126 ± 0.038 | 0.120 ± 0.017 | 0.040 ± 0.005 |
| IKAN-direct    | **0.055** ± 0.002 | **0.110** ± 0.039 | **0.118** ± 0.038 | **0.111** ± 0.018 | **0.018** ± 0.004 |
| MIKAN          | **0.055** ± 0.002 | 0.142 ± 0.044 | **0.108** ± 0.029 | **0.108** ± 0.015 | 0.037 ± 0.004 |

Figure 4: Attention weights and RMSE on Housing dataset. (a)-(c): A histogram for attention weights for different $p$, and the weights become sparse when $p = 0.1$. (d) shows the RMSE of MIKAN for each $p$.

#### 4.4 Node Classification

We implement our models and GAT based on PyTorch Geometric [24], and we repeat ten experiments for each dataset. Table 4 represents the average accuracy and standard deviations. Figure 5a and 5b shows the spectral density in GAT and MIKAN by using t-SNE [25], respectively. The scaled dot-product attention depends on the RBF kernel, and its spectral density is fixed as a Gaussian distribution. However, MIKAN estimates the spectral density depending on the dataset. Figure 5c shows the learned full covariance $\Sigma$ in $q_c$ of MIKAN, and Figure 5d represents the standard deviation of attention weights across the heads. The results support that MIKAN has relatively diverse attention weights across the heads by imposing the dependency between heads with the copula.

### Table 4: Accuracy for the node classification task.

| Method       | Cora    | Citepeer | Pubmed |
|--------------|---------|----------|--------|
| MLP          | 55.1%   | 46.5%    | 71.4%  |
| ManiReg [26] | 59.5%   | 60.1%    | 70.7%  |
| SemiEmb [27] | 59.0%   | 59.6%    | 71.7%  |
| LP [28]      | 68.0%   | 45.3%    | 63.0%  |
| DeepWalk [29]| 67.2%   | 43.2%    | 65.3%  |
| ICA [30]     | 75.1%   | 69.1%    | 73.9%  |
| Planetoid [31]| 75.7%  | 64.7%    | 77.2%  |
| Chebyshev [32]| 81.2%  | 69.8%    | 74.4%  |
| GAT [6]      | 83.1 ± 0.5% | 71.4 ± 0.5% | 78.1 ± 0.6% |
| GAT (scaled dot) | 83.0 ± 0.5% | 71.6 ± 0.5% | 78.2 ± 0.8% |
| IKAN-direct  | 83.3 ± 0.5% | 71.9 ± 0.7% | **78.6 ± 0.3%** |
| MIKAN        | **83.4 ± 0.6%** | **71.9 ± 0.5%** | 78.3 ± 0.5% |

Figure 5: MIKAN estimates $w$ adaptively (b), and shows relatively diverse attention across each head (d) by introducing the copula augmentation (c).

#### 5 Conclusion

This work provides the new interpretation of the scaled dot-product attention as a product of similarity with kernel and magnitude with $L^2$ norm. We analyze the property of kernel and norm in the scaled dot-product attention theoretically and empirically. From the derivation, we generalize the scaled-dot product attention with an implicit kernel function and $L^p$ norm. Furthermore, we propose the copula-augmented spectral density estimation for dependency modeling in MHA. We apply our models to Transformer and GAT, and validate the performance on extensive experiments.
Broader Impact

We generalize the scaled dot-product attention, and we believe that our model is useful for capturing the underlying pattern or context of the given dataset. Context modeling helps us to understand the abstract meaning of data, such as a sentence or user behavior. We expect that our proposed models contribute both machine learning and social science. For the machine learning society, attention is widely used in many domains, such as natural language processing and vision. We make a new direction to improve the scaled dot-product attention. There are many ways to improve attention based on our direction. Many theoretical and empirical analyses of the kernel have been conducted, and we can apply the kernel-related technique, such as inducing points to the attention. Besides, our work can be further extended to be the more generalized data-adaptive norm instead of $L^p$ norm and hyper-parameter $p$. For the social science aspect, we can apply our model to the recommendation, psychotherapy, and political ideal point estimation of legislators by capturing the context or patterns of user log history. On the other hand, identifying underlying patterns that the user does not want might cause a privacy issue. If we adopt guided attention or context modeling that guides the model to attend or not, it can alleviate the privacy issue a bit.

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