Rethinking and Improving Relative Position Encoding for Vision Transformer

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Abstract

Relative position encoding (RPE) is important for transformer to capture sequence ordering of input tokens. General efficacy has been proven in natural language processing. However, in computer vision, its efficacy is not well studied and even remains controversial, e.g., whether relative position encoding can work equally well as absolute position? In order to clarify this, we first review existing relative position encoding methods and analyze their pros and cons when applied in vision transformers. We then propose new relative position encoding methods dedicated to 2D images, called image RPE (iRPE). Our methods consider directional relative distance modeling as well as the interactions between queries and relative position embeddings in self-attention mechanism. The proposed iRPE methods are simple and lightweight. They can be easily plugged into transformer blocks. Experiments demonstrate that solely due to the proposed encoding methods, DeiT [21] and DETR [1] obtain up to 1.5% (top-1 Acc) and 1.3% (mAP) stable improvements over their original versions on ImageNet and COCO respectively, without tuning any extra hyperparameters such as learning rate and weight decay. Our ablation and analysis also yield interesting findings, some of which run counter to previous understanding. Code and models are open-sourced at https://github.com/microsoft/Cream/tree/main/iRPE.

1. Introduction

Transformer recently has drawn great attention in computer vision because of its competitive performance and superior capability in capturing long-range dependencies [1, 2, 7, 21, 24]. The core of transformer is self-attention [22], which is capable of modeling the relationship of tokens in a sequence. Self-attention, however, has an inherent deficiency — it cannot capture the ordering of input tokens. Therefore, incorporating explicit representations of position information is especially important for transformer, since the model is otherwise entirely invariant to sequence ordering, which is undesirable for modeling structured data.

There are mainly two classes of methods to encode positional representations for transformer. One is absolute, while the other is relative. Absolute methods [8, 22] encode the absolute positions of input tokens from 1 to maximum sequence length. That is, each position has an individual encoding vector. The encoding vector is then combined with the input token to expose positional information to the model. On the other hand, relative position methods [4, 17] encode the relative distance between input elements and learn the pairwise relations of tokens. Relative position encoding (RPE) is commonly calculated via a look-up table with learnable parameters interacting with queries and keys in self-attention modules [17]. Such scheme allows the modules to capture very long dependencies between tokens. Relative position encoding has been verified to be effective in natural language processing [4, 6, 15, 25]. However, in computer vision, the efficacy is still unclear. There are few recent works [3, 7, 18] shedding light on it, but obtaining controversial conclusions in vision transformers. For example, Dosovitskiy *et al.* [7] observed that the relative position encoding does not bring any gain comparing to the absolute one (please refer to Tab. 8 in [7]). On the contrary, Srinivas *et al.* [18] found that relative position encoding can induce an apparent gain, being superior to the absolute one (please refer to Tab. 4 in [18]). Moreover, the mostly recent work [3] claims that the relative positional encoding cannot work equally well as the absolute ones (please refer to Tab. 5 in [3]). These works draw different conclusions on the effectiveness of relative position encoding in models, that motivates us to rethink and improve the usage of relative positional encoding in vision transformer.

On the other hand, the original relative position encoding is proposed for language modeling, where the input data is 1D word sequences [4, 17, 22]. But for vision tasks, the inputs are usually 2D images or video sequences, where the pixels are highly spatially structured. It is unclear that:

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whether the naive extension from 1D to 2D is suitable for vision models; whether the directional information is important in vision tasks?

In this paper, we first review existing relative position encoding methods, and then propose new methods dedicated to 2D images. We make the following contributions.

- We analyze several key factors in relative position encoding, including the relative direction, the importance of context, the interactions between queries, keys, values and relative position embeddings, and computational cost. The analysis presents a comprehensive understanding of relative position encoding, and provides empirical guidelines for new method design.
- We introduce an efficient implementation of relative encoding, which reduces the computational cost from the original $\mathcal{O}(n^2d)$ to $\mathcal{O}(nkd)$, where $k \ll n$. Such implementation is suitable for high-resolution input images, such as object detection and semantic segmentation, where the token number might be very large.
- We propose four new relative position encoding methods, called image RPE (iRPE), dedicated to vision transformers, considering both efficiency and generalizability. The methods are simple and can be easily plugged into self-attention layers. Experiments show that, without adjusting any hyperparameters and settings, the proposed methods can improve DeiT-S [21] and DETR-ResNet50 [1] by 1.5% (top-1 Acc) and 1.3% (mAP) over their original models on ImageNet [5] and COCO [12], respectively.
- We answer previous controversial questions. We empirically demonstrate that relative position encoding can replace the absolute encoding for image classification task. Meanwhile, the absolute encoding is necessary for object detection, where the pixel position is important for object localization.

2. Background

2.1. Self-Attention

Self-attention plays a fundamental role in transformer. It maps a query and a set of key-value pairs to an output. More specifically, for an input sequence, *e.g.*, the embeddings of words or image patches, $\mathbf{x} = (\mathbf{x}_1, \dots, \mathbf{x}_n)$ of n elements where $\mathbf{x}_i \in R^{d_x}$, self-attention computes an output sequence $\mathbf{z} = (\mathbf{z}_1, \dots, \mathbf{z}_n)$ where $\mathbf{z}_i \in \mathbb{R}^{d_z}$. Each output element $\mathbf{z}_i$ is computed as a weighted sum of input elements:

$$\mathbf{z}_i = \sum_{j=1}^{n} \alpha_{ij} (\mathbf{x}_j \mathbf{W}^V). \tag{1}$$

Each weight coefficient α_{ij} is computed using a softmax:

$$\alpha_{ij} = \frac{\exp(e_{ij})}{\sum_{k=1}^{n} \exp(e_{ik})}, \tag{2}$$

where e_{ij} is calculated using a scaled dot-product attention:

$$e_{ij} = \frac{(\mathbf{x}_i \mathbf{W}^Q)(\mathbf{x}_j \mathbf{W}^K)^T}{\sqrt{d_z}}. \tag{3}$$

Here, the projections $\mathbf{W}^Q$, $\mathbf{W}^K$, $\mathbf{W}^V \in \mathbb{R}^{d_x \times d_z}$ are parameter matrices, which are unique per layer.

Rather than computing the self-attention once, Multi-head self-attention (MHSA) [22] runs the self-attention multiple times in parallel, *i.e.*, employing h attention heads. The attention head outputs are simply concatenated and linearly transformed into the expected dimensions.

2.2. Position Encoding

Absolute Position Encoding. Since transformer contains no recurrence and no convolution, in order for the model to make use of the order of the sequence, we need to inject some information about the position of the tokens. The original self-attention considers the *absolute position* [22], and add the absolute positional encodings $\mathbf{p} = (\mathbf{p}_1, \dots, \mathbf{p}_n)$ to the input token embedding $\mathbf{x}$ as

$$\mathbf{x}_i = \mathbf{x}_i + \mathbf{p}_i, \tag{4}$$

where the positional encoding $\mathbf{p}_i, \mathbf{x}_i \in \mathcal{R}^{d_x}$. There are several choices of absolute positional encodings, such as the fixed encodings by sine and cosine functions with different frequencies and the learnable encodings through training parameters [8, 22].

Relative Position Encoding. Besides the absolute position of each input element, recent works also consider the pairwise relationships between elements, *i.e.*, *relative position* [17]. Relative relation is presumably important for tasks where the relative ordering or distance of the elements matters. This type of methods encode the relative position between the input elements $\mathbf{x}_i$ and $\mathbf{x}_j$ into vectors $\mathbf{p}^V_{ij}$, $\mathbf{p}^Q_{ij}$, $\mathbf{p}^K_{ij} \in \mathbb{R}^{d_z}$, where $d_z = d_x$. The encoding vectors are embedded into the self-attention module, which re-formulates Eq. (1) and Eq. (3) as

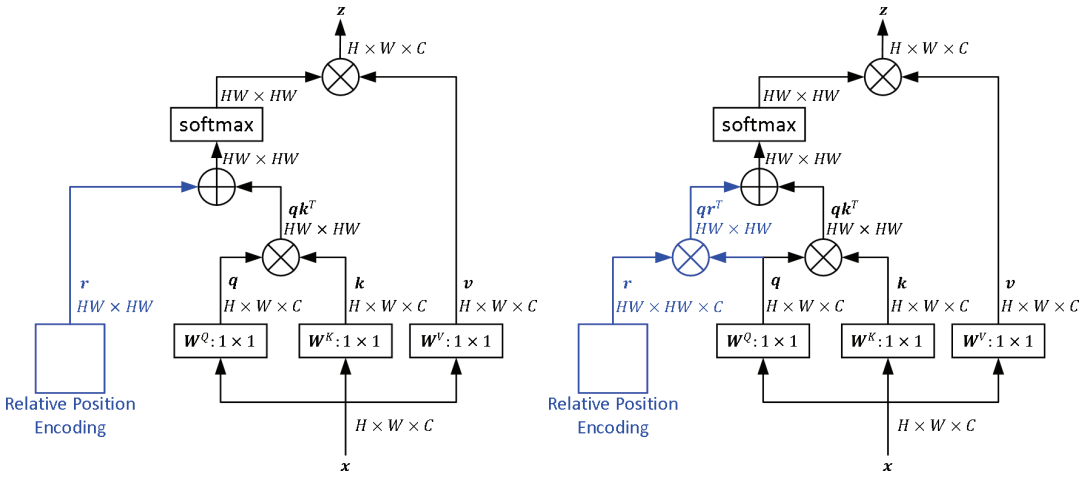
$$\mathbf{z}_i = \sum_{j=1}^{n} \alpha_{ij} (\mathbf{x}_j \mathbf{W}^V + \mathbf{p}^V_{ij}), \tag{5}$$

$$e_{ij} = \frac{(\mathbf{x}_i \mathbf{W}^Q + \mathbf{p}^Q_{ij})(\mathbf{x}_j \mathbf{W}^K + \mathbf{p}^K_{ij})^T}{\sqrt{d_z}}. \tag{6}$$

In this fashion, the pairwise positional relation is learned during transformer training. Such relative position encoding can be either shared across attention heads or not.

3. Method

In this section, we first review previous relative position encoding methods and analyze their differences. Then, we propose four new methods dedicated to vision transformer, and their efficient implementation.



(a) bias mode (b) contextual mode

Figure 1: Illustration of self-attention modules with 2D relative position encoding on keys. The blue parts are newly added.

3.1. Previous Relative Position Encoding Methods

Shaw's RPE. Shaw *et al.* [17] propose a relative position encoding for self-attention. The input tokens are modeled as a directed and fully-connected graph. Each edge between two arbitrary positions i and j is presented by a learnable vector $\mathbf{p}_{ij} \in \mathbb{R}^{d_z}$, namely relative position encoding. Besides, the authors deemed that precise relative position information is not useful beyond a certain distance, so introduced a clip function to reduce the number of parameters. The encoding is formulated as

$$\mathbf{z}_i = \sum_{j=1}^{n} \alpha_{ij}(\mathbf{x}_j\mathbf{W}^V + \mathbf{p}^V_{clip(i-j,k)}), \tag{7}$$

$$e_{ij} = \frac{(\mathbf{x}_i\mathbf{W}^Q)(\mathbf{x}_j\mathbf{W}^K + \mathbf{p}^K_{clip(i-j,k)})^T}{\sqrt{d_z}}, \tag{8}$$

$$clip(x,k) = max(-k, min(k,x)), \tag{9}$$

where $\mathbf{p}^V$ and $\mathbf{p}^K$ are the trainable weights of relative position encoding on values and keys, respectively. $\mathbf{p}^V = (\mathbf{p}^V_{-k}, ..., \mathbf{p}^V_k)$ and $\mathbf{p}^K = (\mathbf{p}^K_{-k}, ..., \mathbf{p}^K_k)$ where $\mathbf{p}^V_i, \mathbf{p}^K_i \in \mathbb{R}^{d_z}$. The scalar k is the maximum relative distance.

RPE in Transformer-XL. Dai *et al.* [4] introduce additional bias terms for queries, and uses the sinusoid formulation for relative position encoding, which is formulated as

$$e_{ij} = \frac{(\mathbf{x}_i\mathbf{W}^Q + \mathbf{u})(\mathbf{x}_j\mathbf{W}^K)^T + (\mathbf{x}_i\mathbf{W}^Q + \mathbf{v})(\mathbf{s}_{i-j}\mathbf{W}^R)^T}{\sqrt{d_z}}, \tag{10}$$

where $\mathbf{u}, \mathbf{v} \in \mathbb{R}^{d_z}$ are two learnable vectors.

The sinusoid encoding vector $\mathbf{s}$ provides the prior of relative position [22]. $\mathbf{W}^R \in \mathbb{R}^{d_z \times d_z}$ is a trainable matrix, projecting $\mathbf{s}_{i-j}$ into a location-based key vector.

Huang's RPE. Huang *et al.* [11] propose a new method considering the interactions of queries, keys and relative positions simultaneously. The equation is given as follows

$$e_{ij} = \frac{(\mathbf{x}_i\mathbf{W}^Q + \mathbf{p}_{ij})(\mathbf{x}_j\mathbf{W}^K + \mathbf{p}_{ij})^T - \mathbf{p}_{ij}\mathbf{p}_{ij}^T}{\sqrt{d_z}}, \tag{11}$$

where $\mathbf{p}_{ij} \in \mathbb{R}^{d_z}$ is the relative position encoding shared by queries and keys.

RPE in SASA. The above three methods are all designed for 1D word sequence in language modeling. Ramachandran *et al.* [16] propose an encoding method for 2D images. The idea is simple. It divides the 2D relative encoding into horizontal and vertical directions, such that each direction can by modeled by a 1D encoding. The method formulation is given as follows

$$e_{ij} = \frac{(\mathbf{x}_i\mathbf{W}^Q)(\mathbf{x}_j\mathbf{W}^K + concat(\mathbf{p}^K_{\delta\tilde{x}}, \mathbf{p}^K_{\delta\tilde{y}}))^T}{\sqrt{d_z}}, \tag{12}$$

where $\delta\tilde{x} = \tilde{x}_i - \tilde{x}_j$ and $\delta\tilde{y} = \tilde{y}_i - \tilde{y}_j$ denote the relative position offsets on x-axis and y-axis of the image coordinate respectively, $\mathbf{p}^K_{\delta\tilde{x}}$ and $\mathbf{p}^K_{\delta\tilde{y}}$ are learnable vectors with length $\frac{1}{2}d_z$, the *concat* operation concatenates the two encodings to form a final relative encoding with length of d_z. In other words, the same offsets on x-axis or y-axis share the same relative position encoding, so this method is able to reduce the number of learnable parameters and computational cost. However, the encoding is only applied on keys. In our experiments, we observe that the RPE imposed on keys, queries and values simultaneously is the most effective one, as presented in Tab. 4 and Tab. 5.

RPE in Axial-Deeplab. Wang *et al.* [23] introduce a position-sensitive method that adds qkv-dependent positional bias into self-attention. The position sensitivity is applied on axial attention that propagates information along height-axis and width-axis sequentially. However, when the relative distance is larger than a threshold, the encoding is set to zero. We observe that long-range relative position information is useful, as analysed in Tab. 6. The position-sensitivity might be competitive when imposed on the standard self-attention. If equipped with the proposed piecewise function, it can be further improved and become more efficient for modeling long-range dependencies.

3.2. Proposed Relative Position Encoding Methods

We design our image RPE (iRPE) methods to analyze several factors which are not well studied in prior works (see the analysis in Sec. 4.2). First, to study whether the encoding can be independent of the input embeddings, we introduce two relative position modes: bias and contextual. We present a piecewise function to map relative positions to encodings, being different from the conventional clip function. After that, to study the importance of directivity, we design two undirected and two directed methods. Finally we provide an efficient implementation for our methods.

Bias Mode and Contextual Mode. Previous relative position encoding methods all depend on input embeddings. It brings a question, *i.e.*, whether the encoding can be independent of the input? We introduce bias mode and contextual mode of relative position encoding to study the question. The former one is independent of input embeddings, while the latter one considers the interaction with queries, keys or values. More specifically, we introduce a unified formulation as

$$e_{ij} = \frac{(\mathbf{x}_i \mathbf{W}^Q)(\mathbf{x}_j \mathbf{W}^K)^T + b_{ij}}{\sqrt{d_z}}, \tag{13}$$

where $b_{ij} \in \mathbb{R}$ is the 2D relative position encoding, defining the bias or contextual mode. For bias mode,

$$b_{ij} = r_{ij}, \tag{14}$$

where $r_{ij} \in \mathbb{R}$ is a learnable scalar and represents the relative position weight between the position i and j. For contextual mode,

$$b_{ij} = (\mathbf{x}_i \mathbf{W}^Q)\mathbf{r}_{ij}{}^T, \tag{15}$$

where $\mathbf{r}_{ij} \in \mathbb{R}^{d_z}$ is a trainable vector, interacted with the query embedding. There are multiple variants for b_{ij} in contextual mode. For example, the relative position encoding operated on both queries and keys can be presented as

$$b_{ij} = (\mathbf{x}_i \mathbf{W}^Q)(\mathbf{r}^K_{ij})^T + (\mathbf{x}_j \mathbf{W}^K)(\mathbf{r}^Q_{ij})^T, \tag{16}$$

where $\mathbf{r}^K_{ij}, \mathbf{r}^Q_{ij} \in \mathbb{R}^{d_z}$ are both learnable vectors. Besides, contextual mode can also be applied on value embeddings,

$$\mathbf{z}_i = \sum_{j=1}^{n} \alpha_{ij}(\mathbf{x}_j \mathbf{W}^V + \mathbf{r}^V_{ij}), \tag{17}$$

where $\mathbf{r}^V_{ij} \in \mathbb{R}^{d_z}$. The relative position weights $\mathbf{r}^Q_{ij}$, $\mathbf{r}^K_{ij}$ and $\mathbf{r}^V_{ij}$ can be constructed in the same way. For a unified representation, we use $\mathbf{r}_{ij}$ to denote them in bias mode and contextual mode in the following discussion. Fig. 1 shows the illustration of self-attention modules with 2D relative position encoding on keys in the propsoed two modes.

A Piecewise Index Function. Before describing the 2D relative position weight $\mathbf{r}_{ij}$, we first introduce a many-to-one function, mapping a relative distance into an integer in finite set, then $\mathbf{r}_{ij}$ can be indexed by the integer and share encondings among different relation positions. Such index function can largely reduce computation costs and the number of parameters for long sequence (*e.g.*, high resolution images). Although the clip function $h(x) = max(-\beta, min(\beta, x))$ used in [17] also reduces the cost, the positions whose relative distance is larger than β are assigned to the same encoding. This method inevitably drops out the contextual information of long-range relative positions. Inspired by [15], we introduce a piecewise function $g(x) : \mathbb{R} \to \{y \in \mathbb{Z} | -\beta \leq y \leq \beta\}$ for indexing relative distances to corresponding encodings. The function is based on a hypothesis that the closer neighbors are more important than the further ones, and distributes the attention by the relative distance. It is presented as

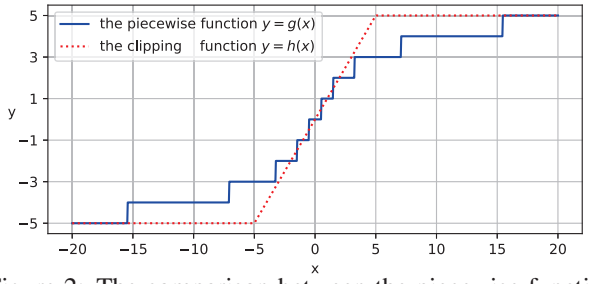


Figure 2: The comparison between the piecewise function $g(x)$ and the clip function $h(x)$.

$$g(x) = \begin{cases} [x], & |x| \leq \alpha \\ sign(x) \times min(\beta, [\alpha + \frac{\ln(|x|/\alpha)}{\ln(\gamma/\alpha)}(\beta - \alpha)]), & |x| > \alpha \end{cases} \tag{18}$$

where $[\cdot]$ is a round operation, $sign(x)$ determines the sign of a number, *i.e.*, returning 1 for positive input, -1 for negative, and 0 for otherwise. α determines the piecewise point, β controls the output in the range of $[-\beta, \beta]$, and γ adjusts the curvature of the logarithmic part.

We compare the piecewise function $g(x)$ with the clip function $h(x) = min(-\beta, max(\beta, x))$, *i.e.* Eq. (9). In Fig. 2, the clip function $h(x)$ distributes uniform attention and leaves out long distance positions, but the piecewise function $g(x)$ distributes different levels of attention by relative distance. We suppose that the potential information in long-range position should be preserved, especially for high resolution images or the tasks requiring long-range feature dependencies, so $g(x)$ is selected to construct our mapping method for $\mathbf{r}_{ij}$.

2D Relative Position Calculation. In order to calculate relative position on 2D image plane and define the relative weight $\mathbf{r}_{ij}$, we propose two undirected mapping methods, namely Euclidean and Quantization, as well as two directed mapping methods, namely Cross and Product.

Euclidean method. On image plane, the relative position $(\tilde{x}_i - \tilde{x}_j, \tilde{y}_i - \tilde{y}_j)$ is a 2D coordinate. We compute Euclidean distance between two positions, and maps the distance into the corresponding encoding. The method is undirected and formulated as

$$\mathbf{r}_{ij} = \mathbf{p}_{I(i,j)}, \tag{19}$$

$$I(i,j) = g(\sqrt{(\tilde{x}_i - \tilde{x}_j)^2 + (\tilde{y}_i - \tilde{y}_j)^2}), \tag{20}$$

where $\mathbf{p}_{I(i,j)}$ is either a learnable scalar in bias mode or a vector in contextual mode. We regard $\mathbf{p}_{I(i,j)}$ as a bucket, which stores the relative position weight. The number of buckets is $2\beta+1$, as defined in Eq. (18).

Quantization method. In the above Euclidean method, the closer two neighbors with different relative distances may be mapped into the same index, e.g. the 2D relative positions (1, 0) and (1, 1) are both mapped into the index 1. We suppose that the close neighbors should be separated. Therefore, we quantize Euclidean distance, i.e., different real number is mapped into different integer. We revise $I(i,j)$ in Eq. (19) as

$$I(i,j) = g(quant(\sqrt{(\tilde{x}_i-\tilde{x}_j)^2+(\tilde{y}_i-\tilde{y}_j)^2})). \quad (21)$$

The operation *quant* maps a set of real numbers {0, 1, 1.41, 2, 2.24, ...} into a set of integers {0, 1, 2, 3, 4, ...}. This method is also undirected.

Cross method. Positional direction of pixels is also important for images, we thereby propose directed mapping methods. This method is called Cross method, which computes encoding on horizontal and vertical directions separately, then summarizes them. The method is given as

$$\mathbf{r}_{ij} = \mathbf{p}^{\tilde{x}}_{I^{\tilde{x}}(i,j)} + \mathbf{p}^{\tilde{y}}_{I^{\tilde{y}}(i,j)}, \quad (22)$$

$$I^{\tilde{x}}(i,j) = g(\tilde{x}_i - \tilde{x}_j), \quad (23)$$

$$I^{\tilde{y}}(i,j) = g(\tilde{y}_i - \tilde{y}_j), \quad (24)$$

where $\mathbf{p}^{\tilde{x}}_{I(i,j)}$ and $\mathbf{p}^{\tilde{y}}_{I(i,j)}$ are both learnable scalars in bias mode, or a learnable vectors in contextual mode. Similar to the encoding in SASA [16], the same offsets on x-axis or y-axis share the same encoding, but the main difference is that we use a piecewise function to distribute attention by relative distance. The number of buckets is $2\times(2\beta+1)$.

Product method. The Cross method encodes different relative positions into the same embedding if the distance on one direction is identical, either horizontal or vertical. Besides, the addition operation in Eq. (22) brings extra computational cost. To improve efficiency and involve more directional information, we design Product method which is formulated as

$$\mathbf{r}_{ij} = \mathbf{p}_{I^{\tilde{x}}(i,j),I^{\tilde{y}}(i,j)}. \quad (25)$$

The right side of the equation is a trainable scalar in bias mode, or a trainable vector in contextual mode. $I^{\tilde{x}}(i,j)$ and $I^{\tilde{y}}(i,j)$ are defined in Eq. (23) and Eq. (24), and the combination of them is a 2D index for $\mathbf{p}$. The number of buckets is $(2\beta+1)^2$.

An Efficient Implementation. For the above proposed methods in contextual mode, there is a common term $(\mathbf{x}_i\mathbf{W})\mathbf{p}_{I(i,j)}{}^T$ when putting Eq. (19), Eq. (22) or Eq. (25) into Eq. (15). Let y_{ij} denote the common term as follows,

$$y_{ij} = (\mathbf{x}_i\mathbf{W})\mathbf{p}_{I(i,j)}{}^T. \quad (26)$$

It takes time complexity $\mathcal{O}(n^2d)$ to compute all y_{ij}, where n and d are the length of the input sequence and the number of feature channels, respectively. Due to the many-to-one property of $I(i,j)$, the set size k of $I(i,j)$ is usually less than n in vision transformer. Therefore, we provide an efficient implementation as follows,

$$z_{i,t} = (\mathbf{x}_i\mathbf{W})\mathbf{p}_t{}^T, t \in \{I(i,j)|i,j\in[0,n)\}, \quad (27)$$

$$y_{ij} = z_{i,I(i,j)}. \quad (28)$$

It first takes time complexity $\mathcal{O}(nkd)$ to pre-compute all $z_{i,t}$ by Eq. (27), then assigns $z_{i,t}$ to all y_{ij} by the mapping $t = I(i,j)$ by Eq. (28). The assignment operation takes time complexity $\mathcal{O}(n^2)$, whose cost is much smaller than that of the pre-computation procedure. Thus, the computational cost of relative position encoding reduces from the original $\mathcal{O}(n^2d)$ to $\mathcal{O}(nkd)$.

4. Experiments

In this section, we first provide some analysis by comparing different position embeddings, followed by experiments on the effects of key factors in relative position encoding. Then, we compare the proposed methods with the state-of-the-art methods on image classification and object detection tasks. Finally, we visualize the relative position encoding and explain why it works.

4.1. Implementation Details

We choose the recent vision transformer model DeiT [21] as the baseline for most experiments. The relative position encoding is added into all self-attention layers. If not specified, RPE is only added on keys. We set α:β:γ = 1:2:8 for the piecewise function $g(x)$, and adjust the number of buckets by changing β. An extra bucket is used to store the relative position encodings of the classification token.

For fair comparison, we adopt the same training settings as DeiT [21]: AdamW [13] optimizer with weight decay 0.05, initial learning rate 1x10^{-3} and minimal learning 1x10^{-5} with cosine scheduler, 5 epochs warmup, batch size of 1024, 0.1 label smoothing [19], and stochastic depth with survival rate of 0.9. The images are split into 14x14 non-overlapping patches. Data augmentation methods [26, 27] are consistent with DeiT [21]. All models are trained from scratch for 300 epochs with 8 NVIDIA Tesla V100 GPUs.

4.2. Analysis on Relative Position Encoding

Directed v.s. *Undirected.* As shown in Tab. 1, directed methods (Cross and Product), in general, perform better than undirected ones (Euclidean and Quantization) in vision transformer. This phenomenon illustrates that the directivity is important for vision transformers, because image pixels are highly structured and semantically correlative.

Method based on DeiT-S [21]	Is Directed	Mode	Top-1 Acc(%)	Δ Acc(%)
Original [21]	-	-	79.9	–
Euclidean	×	bias	80.1	+0.2
		contextual	80.4	+0.5
Quantization	×	bias	80.3	+0.4
		contextual	80.5	+0.6
Cross	✓	bias	80.5	+0.6
		contextual	80.8	+0.9
Product	✓	bias	80.5	+0.6
		contextual	80.9	+1.0

Table 1: Ablation of our relative position encoding methods on ImageNet [5]. The original model is DeiT-S [21], which only uses absolute position encoding. We equip the model with the proposed four relative encoding methods, *i.e.*, Eq. (19), Eq. (21), Eq. (22) and Eq. (25) with the best numbers of buckets of 20, 51, 56 and 50 respectively.

Mode	Shared	#Param. (M)	MACs (M)	Top-1 Acc(%)
Bias	×	22.05	4613	80.54 ± 0.06
	✓	22.05	4613	80.05 ± 0.04
Contextual	×	22.28	4659	80.99 ± 0.16
	✓	22.09	4659	80.89 ± 0.04

Table 2: Ablation of shared and unshared relative position encoding across attention heads. The experiments are conducted over DeiT-S [21] on ImageNet [5] with 50 buckets. The models are trained and evaluated by three times.

Bias v.s. *Contextual.* Tab. 1 shows that the contextual mode achieves superior performance to that of bias mode, regardless of which method uses. The underlying reason might be that contextual mode changes the encoding with the input feature while bias mode keeps static.

Shared v.s. *Unshared.* Self-attention contains multiple heads. RPE can be either shared or unshared across different heads. We show the effects of these two schemes in bias and contextual modes in Tab. 2, respectively. For bias mode, the accuracy drops significantly when sharing encoding across heads. By contrast, in contextual mode, the performance gap between two schemes is negligible. Both of them achieve an average top-1 accuracy of 80.9%. We conjecture that different heads need different RPEs to capture different information. In contextual mode, each head computes its own RPE by the Eq. (15) while in bias mode the shared RPE forces all heads to pay the same attention on patches. For parameter-saving, we adopt the share scheme in our final methods.

Piecewise v.s. *Clip.* We compare the efficacy of the piecewise function $g(x)$ defined in Eq. (18) and the clip function $h(x)$ defined in Eq. (9) in Tab. 3. There is a very small, even negligible, performance gap between them in image classification task. However, in object detection task, we found the clip function is worse than the piecewise one

Function	Mode	Top-1 Acc(%)	Top-5 Acc(%)
clip	bias	80.1	94.9
	contextual	80.9	95.5
piecewise	bias	80.0	95.0
	contextual	80.9	95.5

Table 3: Ablation for clip function and piecewise function. The experiments are conducted over DeiT-S [21] model with product shared-head relative position encoding on ImageNet [5]. The number of buckets is 50.

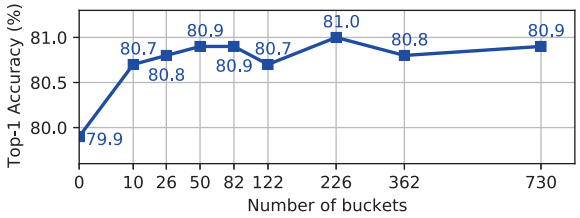


Figure 3: Ablation for the number of buckets in contextual product model with shared RPEs on ImageNet [5].

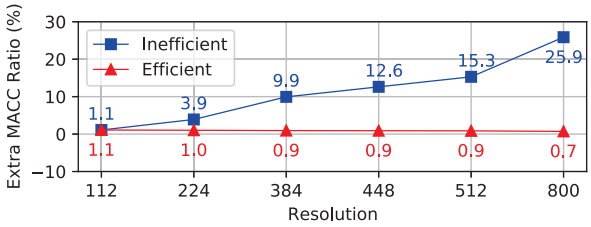


Figure 4: The extra computational cost of RPE with 50 buckets in different implementations under different resolutions. The baseline model is DeiT-S [21]. MACs means multiply-accumulate operations.

as illustrated in Tab. 6 (#5 *v.s.* #6). The underlying reason is that they are similar when the sequence is short. The piecewise function is effective especially when the sequence size is much larger than the number of buckets. Object detection uses a much higher resolution input compared to classification, leading to a much longer input sequence. We therefore conjecture that when the input sequence is long, the piecewise function should be used since it is able to distribute different attentions to the positions with relative large distance, while the clip function assigns the same encoding when the relative distance is larger than β.

Number of buckets. The number of buckets largely affects model parameters, computational complexity and performance. In order to find a balance, we explore the influence of varying the number of buckets for the contextual Product method. Fig. 3 shows the change of top-1 accuracy along with the number of buckets. The accuracy increases from 79.9 to 80.9 before 50 buckets. After that, there is no significant improvement. It shows that the number of buckets 50 is a good balance between the computational cost and the accuracy for 14×14 feature map in DeiT-S [21].

#	Abs Pos.	p_{ij}^Q	p_{ij}^K	p_{ij}^V	Top-1	Top-5
1 [21]	learnable	×	×	×	79.9	95.0
2	×	×	×	×	77.6(-2.3)	93.8
3	×	✓	×	×	80.9(+1.0)	95.4
4	×	×	✓	×	80.9(+1.0)	95.3
5	×	×	×	✓	80.2(+0.3)	95.0
6	×	✓	✓	×	81.0(+1.1)	95.5
7	×	✓	✓	✓	81.3(+1.4)	**95.7**
8	learnable	✓	×	×	80.9(+1.0)	95.5
9	learnable	×	✓	×	80.9(+1.0)	95.5
10	learnable	×	×	✓	80.2(+0.3)	95.1
11	learnable	✓	✓	×	81.1(+1.2)	95.4
12	learnable	✓	✓	✓	**81.4**(+1.5)	95.6

Table 4: Component-wise analysis on ImageNet [5]. We add contextual product shared-head RPE into DeiT-S [21]. The number of buckets is 50. Abs Pos. represents the absolute position encoding. p_{ij}^Q, p_{ij}^K and p_{ij}^V present relative position encodings on queries, keys and values.

Component-wise analysis. We perform a component-wise analysis to study the effects of different position encodings for vision transformer models. We select DeiT-S model [21] as the baseline, and only change the position encoding methods. The learnable absolute position encoding is used in the original model. The relative position encodings are computed by contextual Product method with 50 buckets. The conclusions we got from Tab. 4 are as follows: 1) Removing absolute position encoding from original DeiT-S will cause that the Top-1 accuracy drops from 79.9 to 77.6 (#1 *v.s.* #2). 2) The models with only relative position encoding surpass the one with only absolute position encoding (#3-5 *v.s.* #1). It shows that RPE works well as the absolute one. 3) When equipped with RPE, the absolute one does not bring any gains (#3-5 *v.s.* #8-10). We suppose that the local information is more important than the global one in classification task. 4) The RPE on queries or keys brings more gain than that on values (#3,4 *v.s.* #5). 5) The combination of the encodings on queries, keys and values brings further improvements (#6,7,11,12 *v.s.* others).

Complexity Analysis. We evaluate the computational cost of our proposed methods with respect to different input resolutions. The baseline model is DeiT-S [21] with only absolute position encoding. We adopt contextual product shared-head relative position encoding to the baseline with 50 buckets. Fig. 4 shows our method takes at most 1% extra computational cost with efficient implementation.

4.3. Comparison on Image Classification

We compare our proposed methods with the state-of-the-art methods on image classification tasks. We select DeiT [21] as the baseline. We adopt contextual Product shared-head method with 50 buckets. As shown in Tab. 5, our method brings improvement on all three DeiT models. In particular, we improve the DeiT-Ti/S/B models by 1.5%/1.0%/0.6% respectively, through adding RPE only on keys. We show that the models could be further improved by adding the proposed RPE on both queries and values. When compared with other methods, ours achieve superior performance with less parameters and MACs.

Model	#Param.	Input	MACs (M)	Top-1 Acc (%)
Convnets				
ResNet-50 [10]	25M	224^2	4121	79.0
RegNetY-4.0GF [14]	21M	224^2	4012	79.4
EfficientNet-B1 [20]	8M	240^2	712	79.1
EfficientNet-B5 [20]	30M	456^2	10392	83.6
Transformers				
ViT-B/16 [7]	86M	384^2	55630	77.9
ViT-L/16 [7]	307M	384^2	191452	76.5
DeiT-Ti [21]	5M	224^2	1261	72.2
CPVT-Ti(0-5) [3]	6M	224^2	1262	73.4
DeiT-Ti with iRPE-K(**Ours**)	6M	224^2	1284	73.7
DeiT-S [21]	22M	224^2	4613	79.9
CPVT-S(0-5) [3]	23M	224^2	4616	80.5
DeiT-S(Shaw's) [17, 21]$^+$	22M	224^2	4659	80.9
DeiT-S(Trans.-XL's) [4, 21]$^+$	23M	224^2	4828	80.8
DeiT-S(Huang's) [11, 21]$^+$	22M	224^2	4706	81.0
DeiT-S(SASA's) [16, 21]*	22M	224^2	4639	80.8
DeiT-S with iRPE-K(**Ours**)	22M	224^2	4659	80.9
DeiT-S with iRPE-QK(**Ours**)	22M	224^2	4706	81.1
DeiT-S with iRPE-QKV(**Ours**)	22M	224^2	4885	81.4
DeiT-B [21]	86M	224^2	17592	81.8
CPVT-B(0-5) [3]	86M	224^2	17598	81.9
DeiT-B with iRPE-K(**Ours**)	87M	224^2	17684	82.4

$^+$ We utilize our product method to adapt 1D encoding for 2D images with the clip function. The encoding weight is shared across heads.
* DeiT-S [21] with SASA [16]'s relative position encoding.

Table 5: Comparison on ImageNet [5].

4.4. Comparison on Object Detection

To verify the generality, we further evaluate our method on COCO 2017 detection dataset [12]. We use the transformer-based detection model DETR [1] as baseline, and follow the same train/val settings (including hyperparameters), except injecting RPE into all self-attention modules in the encoder. As shown in Tab. 6 (#1,6 and #8,9), our method consistently improve the performance of DETR by 1.3 and 1.7 mAP under 150 and 300 training epochs.

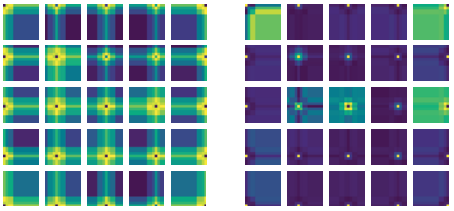
In addition, we conduct ablation studies analyzing that the effects of position encoding on object detection task. Comparing #1, #2 and #4 in Tab. 6, we give the conclusion that position encoding is crucial for DETR. We also show that absolute position embedding is better than relative position embedding in DETR, which is contrast to the observation in classification. We conjecture that DETR needs the prior of absolute position encoding to locate objects.

4.5. Visualization

To explore the underlying reason of relative position encoding, we visualize the extra weights b_{ij} (defined in Eq. (13)) added into the attention by RPE for different po-

#	Abs Pos.	Rel Pos.	#buckets	epoch	AP	AP_{50}	AP_{75}	AP_S	AP_M	AP_L
1 [1]	sinusoid	none	-	150	39.5	60.3	41.4	17.5	43.0	59.1
2	none	none	-	150	30.4(-9.1)	52.5	30.2	9.4	31.2	50.5
3	sinusoid	bias	9×9	150	40.6(+1.1)	61.2	42.8	19.0	43.9	60.2
4	none	contextual	9×9	150	38.7(-0.8)	60.1	40.4	18.2	41.8	56.7
5	sinusoid	ctx clip	9×9	150	40.4(+0.9)	60.9	42.4	19.1	43.7	59.8
6	sinusoid	contextual	9×9	150	40.8(+1.3)	61.5	42.5	18.5	44.4	60.5
7	sinusoid	contextual	15×15	150	40.8(+1.3)	61.7	42.6	18.5	44.2	61.2
8 [1]	sinusoid	none	-	300	40.6	61.6	-	19.9	44.3	60.2
9	sinusoid	contextual	9×9	300	42.3(+1.7)	62.8	44.3	20.7	46.2	61.1

Table 6: Component-wise analysis on DETR [1].



(a) block 0 (b) block 10

Figure 5: Visualization of relative position encoding (RPE) in contextual product method. We show the extra weights added to the attention by RPE for different positions. (a), (b) display the RPE weights for 5×5 reference patches uniformly sampled from 14×14 patches in block 0 and 10.

sitions. From Fig. 5, RPE makes patches focus more on its neighboring patches in block 0. However, when it turns to higher blocks, this phenomenon disappears. We conjecture that after passing through multiple layers, the model has already captured enough local information. The shallow layers in transformer are global attentions, paying attention to the whole image (consisting of small patches). It is different from CNN models in which shallow layers only capture local information. In theory, without RPE (or other additional operations such as local windows), transformer does not explicitly capture locality. RPEs inject Conv-like inductive bias (including locality) into transformer, improving the model capability of capturing local patterns.

5. Related Work

Transformer. Transformer was originally introduced by Vaswani *et al.* [22] for natural language processing, and recently extended to computer vision [1, 7, 21]. In this work we study vision transformers in image classification and object detection tasks, and select DeiT [21] and DETR [1] as our baseline models. In ViT [7] and DeiT [21], an image is split into multiple fixed-size patches. The embedded features of patches are added with absolute position encoding to fed in a standard transformer encoder. An extra trainable classification token is added into the sequence for classification. In DETR [1], a CNN backbone is used for feature extraction first. Its output, a $32\times$ downsampling feature map is flatten and fed in a transformer that outputs a certain number of bounding boxes. A learnable or sinusoid absolute position encoding is added in encoder and decoder.

Relative Position Encoding. Relative position encoding is proposed firstly by Shaw *et al.* [17], where relative position encodings are added into keys and values. Dai *et al.* [4] proposed relative position encoding with the prior of the sinusoid matrix and more learnable parameters. Huang *et al.* [11] proposed several 1D encoding variants. The effectiveness of relative position encoding has been verified in natural language processing. There are also some works utilizing relative position encoding on 2D visual tasks. Ramachandran *et al.* [16, 18] proposed 2D relative position encoding that computes and concatenates separate encodings of each dimension. Chu *et al.* [3] proposed position encoding generator, inserted between encoders. However, the efficacy of relative position encoding in visual transformer is still unclear, which is discussed and addressed in this work.

6. Conclusions and Remarks

In this paper, we review existing relative position encoding methods, and propose four methods dedicated to visual transformers. The abundant experiments show that our methods bring a clear improvement on both classification and detection tasks with negligible extra complexity. Our methods could be easily plugged into the self-attention modules in vision models. In addition, we give comparison of different methods and analysis on RPE with following conclusions. 1) RPE can be shared among different heads for parameter-saving. It is able to achieve comparable performance with the non-shared one in contextual mode. 2) RPE can replace the absolute one in image classification task. However, absolute position encoding is necessary for object detection task, which needs to predict locations of objects. 3) RPE should consider the positional directivity, which is important to structured 2D images. 4) RPE forces the shallow layers to pay more attention to local patches.

In future work, we plan to extend our method to other attention-based models and scenarios, such as high-resolution input tasks like semantic segmentation [29], and non-pixel input tasks like point cloud classification [9, 28].

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