LieRE: Generalizing Rotary Position Encodings

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Abstract

While Rotary Position Embeddings (RoPE) for natural language performs well and has become widely adopted, its adoption for other modalities has been slower. Here, we introduce Lie group Relative position Encodings (LieRE) that goes beyond RoPE in supporting higher dimensional inputs. We evaluate the performance of LieRE on 2D and 3D image classification tasks and observe that LieRE leads to marked improvements in performance (up to 6%), training efficiency (3.5x reduction), data efficiency (30%) compared to the baselines of RoFormer, DeiT III, RoPE-Mixed and Vision-Llama.

1 Introduction

While the attention mechanism has achieved widespread use, especially as part of the transformer architecture, attention is invariant to the order of its inputs and requires another mechanism to capture positional information of input tokens [25]. This has spurred a line of work in the subarea of positional encodings—methods of encoding positional information for attention mechanisms.

In particular, Rotary Position Encoding (RoPE) has emerged as a powerful technique for encoding relative positional information in transformer-based models [21]. RoPE's ability to capture relative position information has made it a popular choice for open-source foundation models such as LLaMA. In particular, RoPE implicitly captures *relative* positions. When the token in position x attends to a token in position y, the effect of RoPE depends on $x - y$.

Despite the success of RoPE in sequence tasks, it is designed for one-dimensional sequence data. This has resulted in slow adoption for modalities with higher dimensional data, such as 2D images, and 3D medical images or data that includes a temporal dimension like videos or Electronic Health Records. Furthermore works that do attempt attempt to generalize RoPE to these modalities typically do so with a method tailored specifically to the modality at hand.

Our work aims to answer the question of whether there is a single relative position encoding scheme that well works across modalities of varying dimensions. If possible, this would enable the use of a common model backbone across a much larger variety of tasks.

1.1 Contributions

We introduce Lie Relative Encodings (LieRE), a mechanism that allows the attention mechanism to learn how to utilize relative spatial information in its inputs. We show that LieRE is effective, without modification, across modalities and input dimensionality by evaluating it on both 2D and 3D classification tasks. Beyond improving classification accuracy, LieRE also reduces the amount of

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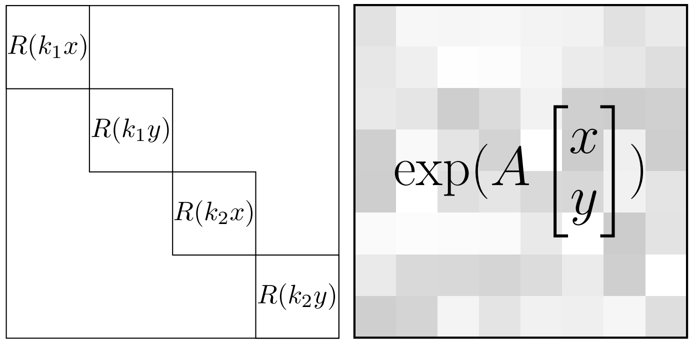


(a) 2D RoPE (b) LieRE

Figure 1: Rotation matrices for a token generated from an image patch. x, y denote the location of the patch from which the token was generated.

computing and data required during training. On the CIFAR100 task, this translates to 3.5x fewer training steps to achieve the same accuracy as the DeiT III baseline and outperforming the DeiT baseline trained on the full set with only a 70% subset of the data. Furthermore, LieRE is simple to implement and adapt to new modalities, requiring only a tokenizer that also outputs a position in $\mathbb{R}^d$ in addition to a standard embedding. In order to aid the reproducibility of our results we will post our code on github.

1.2 Related Work

1.2.1 Position Encodings

The development of various position encodings has been ongoing since the original development of the attention mechanisms. There are three broad classes of positional encodings: 1) absolute 2) relative and 3) contextual.

Absolute encodings generally operate on a per token-level, modifying the embedding of a token to encode the location of the token in the text or media. Classic methods such as sinusoidal embeddings of learned embeddings achieve this by adding either a learned or carefully designed vector to the embedding of the token before it is passed through the transformer [25, 6, 8]. Absolute position measures position with respect to an absolute reference, such as the start of the text or the top left corner of an image.

Relative embeddings are focused on discarding the absolute coordinate system of absolute position encodings and encoding the relative positions of two tokens. This is particularly useful for images, where translation invariance can improve performance, but also widely used for text as well. The original relative position encodings modified the attention mechanism between two tokens with the difference in the positions of two tokens [18, 15, 14]. However, this incurs quadratic computational complexity as an additional operation for every pair of tokens. Rotary Position Encodings (RoPE) avoid this penalty by utilizing the commutativity and orthogonality of 2D rotations. The keys and queries are rotated by a set of 2D rotations before computing the inner product, avoiding the quadratic blowup of earlier relative position schemes. The angle of these rotations depends on the position of the original token. The algebraic properties of attention and 2D rotation matrices ensure that the attention mechanism only depends on the relative positions of the tokens when they attend to each other [21]. RoPE is quite widely used in open source LLMs including the PaLM, Llama and Mixtral models [24, 2, 12]. However, RoPE can perform poorly on inference for larger context sizes than the model was trained on.

We refer to the last category of positional as *contextual* position embeddings. This category is defined by encodings that aim to capture semantic positional information lost in traditional absolute and relative position encodings, often motivated by reasoning or mathematical tasks. Contextual Position encodings achieve (CoPE) this by allowing the model to learn how the position is computed [10]. Abacus embeddings enable transformers to learn how to handle arithmetic by better exposing the digit structure of numbers [16].

1.2.2 Extensions of RoPE

The efficiency and popularity of RoPE have led to several lines of work looking to extend it focused on specific domains.

One notable one is context extension, which aims to address the fact that models trained on short documents tend to perform poorly on long documents. Methods like NTK-aware context extension, YaRN and LongROPE focus on enabling already trained models to handle long context, both with and without finetuning [7, 17].

Another line of work has been specifically focused on adapting RoPE to image tasks. Both VisionLlama and RoPE-Mixed present relative position encodings inspired by RoPE that are able to encode 2D positional data [3, 11] I key difference is that RoPE-Mixed has a learnable component, whereas VisionLlama does not.

2 Background

2.1 Lie Groups in the Context of Attention

In this section, we aim to provide a minimal introduction to Lie groups so that the reader is able to understand the mathematical motivations behind LieRE. Lie groups are very well studied, especially in the context of representation theory and standard texts including [9] are able to provide a more extensive introduction to the subject.

In this context, Lie groups are smooth manifolds that are closed under matrix multiplication and inversion. For every Lie group, the matrix exponential provides a smooth bijective map from a subset of $\mathbb{R}^{n\times n}$ (hereto referred to as the generator set) to the Lie group. The exponential map is a diffeomorphism and has the following key property for generators x, y close together:

$$\exp(x - y) = \exp(-y + x) \approx (\exp(y))^{-1} \exp(x) \tag{1}$$

Section 3.1 will show that this is the key to being able to encode relative positions.

Both RoPE (in the context of text) and RoPE-Mixed use block-diagonal rotation matrices with 2D rotations as blocks. These form a special Lie group that is commutative, allowing us to strengthen the statement in equation (1) to

$$exp(x - y) = exp(x)exp(y)^{-1} = exp(y)^{-1}exp(x). \tag{2}$$

Our work examines the tradeoff between using the stronger property in equation (2) or increased capacity and the weaker property (1). In short, we find that benefit of representational flexibility exceeds the benefit of exactly honoring equation (2).

3 Methods

3.1 Rotations for Relative Positions in Attention

Before introducing the pseudocode we explain how LieRE modifies the attention mechanism and how this relates to Lie groups.

We start by using a linear map to embed the positions as skew-symmetric matrices P_i and P_j and compute high dimensional rotations as $R_i = \exp(P_i)$ and $R_j = \exp(P_j)$.

Recall that, for every pair of tokens, the attention mechanism computes the inner products between their key and query vectors, $k_i^T q_j$. We encode the positions by multiplying by the rotation matrices in the prior part. In particular, we update the keys and queries as $k_i' = k_i R_i$ and $q_j = q_j R_j$. This results in an updated inner product of $(R_i k_i)^T R_j q_j = k_i R_i^T R_j q_j = k_i R_i^{-1} R_j q_j$.

Recall that by equation 1, $R_i^{-1} R_j = \exp(P_i)^{-1} \exp(P_j) \approx \exp(P_j - P_i)$. In other words, the inner product automatically computes the relative position encoding. Note that this is exactly the mechanism behind the original RoPE paper. The difference is that LieRE uses the full set of high dimensional rotations and relaxes the constraint that equation 1 holds with equality. We make the description of the method more precise in the next section.

3.2 LieRE

LieRE modifies the attention mechanism by applying a rotation to the keys and queries before computing their inner products. However, where RoPE applies a block-diagonal $n \times n$ with 2D rotation matrices as blocks, LieRE applies a $n \times n$ rotation matrix. Using the fact that every rotation matrix can be represented as the matrix exponential of a skew-symmetric matrix, we parametrize the rotations with generators before the matrix exponential. This skew-symmetric generator is computed via a learned linear map from the positions to the generator space. Let $x \in \mathbb{R}^n$ indicate the position of the token, and $A : \mathbb{R}^d \to \text{Skew}_n(\mathbb{R})$ be a learnable linear map to the set of skew-symmetric matrices. At the start of every forward pass, we compute the LieRE rotation matrix for each token as

$$R_{LieRE} := \exp(Ax).$$

Then, for each attention mechanism, the keys and queries for a particular token are updated as $\text{key}' := R_{LieRE} \cdot \text{key}, \text{query}' := R_{LieRE} \cdot \text{query}$ We present attention with RoPE and LieRE side by side in algorithms 1 and 2.

Algorithm 1 RoPE Attention (prior work)

procedure ROPE(X, p, d)
  $\theta \leftarrow \frac{1}{10000^{2i/d}} \quad \forall i \in [0, d)$
  for $i \leftarrow 0$ **to** d **step** 2 **do**
    $\text{cos\_pos}_i, \text{sin\_pos}_i \leftarrow \cos(p\theta_i), \sin(p\theta_i)$
    $X_{\text{rotated}}[i] \leftarrow X[i] \cdot \text{cos\_pos}_i - X[i+1] \cdot \text{sin\_pos}_i$
    $X_{\text{rotated}}[i+1] \leftarrow X[i] \cdot \text{sin\_pos}_i + X[i+1] \cdot \text{cos\_pos}_i$
  end for
  return X_{rotated}
end procedure

procedure ROPEATTENTION(Q, K, V)
  $p \leftarrow$ tokenPositions
  $d \leftarrow$ embeddingDimension
  $K_{\text{rotated}} \leftarrow \text{ROPE}(K, p, d)$
  $Q_{\text{rotated}} \leftarrow \text{ROPE}(Q, p, d)$
  Attention $\leftarrow$ softmax$(\frac{Q_{\text{rotated}} K_{\text{rotated}}^T}{\sqrt{d}})V$
  return Attention
end procedure

Algorithm 2 LieRE Attention (our work)

procedure LIERE(X, p, A)
  rotation_matrix $\leftarrow \exp(Ap)$
  $X_{\text{rotated}} \leftarrow X \odot$ rotation_matrix
  return X_{rotated}
end procedure

procedure LIEREATTENTION(Q, K, V, A)
  $p \leftarrow$ tokenPositions
  $K_{\text{rotated}} \leftarrow \text{LIERE}(K, p, A)$
  $Q_{\text{rotated}} \leftarrow \text{LIERE}(Q, p, A)$
  Attention $\leftarrow$ softmax $\left(\frac{Q_{\text{rotated}} K_{\text{rotated}}^T}{\sqrt{\dim(K)}}\right) V$
  return Attention
end procedure

Outside of the generator scaling experiments, we set the rotation dimension equal to the head dimension and apply rotation on a per-attention-head basis.

Note that if we are applying our method to images it is possible to impose a sparsity structure on the generator that recovers RoPE-mixed without the absolute position embeddings [11].

4 Experiments

4.1 Model and Training Parameters

In order to isolate the benefit of LieRE, we use the standard transformer backbone modified to be able to switch between relative position encoding types. The backbone is configured as ViT-B, with 12 layers, a hidden dimension of 768, and an intermediate dimension of 3096. All experiments use dropout of 0.1. All experiments use RandAugment [4].

We avoid using pre-trained weights in order to maximize the comparability of results between methods. All trainers use ADAM with the default parameters for pytorch.

In order to ensure a fair comparison, we explicitly avoid tuning hyperparameters with LieRE and use the same default hyperparameters for all experiments (Appendix A).

4.2 Datasets and Tasks

Our experiments are designed to evaluate the efficacy of LieRE as a position encoding across a diverse set of modalities. We evaluate LieRE on the classification of 2D (images) and 3D (videos and medical images) data. For 3D data and ImageNet (2D), we focus on accuracy. For CIFAR100 (2D), where training is less resource intensive, we also evaluate LieRE's data and training compute efficiency.

4.2.1 2D Classification

For 2D data we evaluate performance on the CIFAR100 and ImageNet image classification task [13, 5]. All hyperparameters and other details necessary for the reproducibility of experiments can be found in appendix A.

We partition our evaluation of performance into four parts. In the first part, we examine accuracy across a range of model architectures on both CIFAR100 and ImageNet. To ensure a fair comparison, we implement all positional encodings on the same [standard] transformer backbone. These experiments are meant to identify the best-performing method of encoding positions.

In the second part, we take advantage of the relatively modest amount of compute resources necessary to train a model for CIFAR 100 to examine LieREs impact on data efficiency. Here we limit our focus to LieRE, RoPE-Mixed, VisionLlama embeddings and absolute position embeddings. We train every model on 30%, 40%,...,90% subsets of CIFAR100 in order to evaluate the sensitivity of each model to the amount of training data. Since training starts to overfit quite early for the smaller datasets, we use the maximum validation accuracy for each run when comparing models.

We also measure training *compute* efficiency by comparing the number of training steps necessary to achieve a fixed level of validation accuracy.

In the third part, we evaluate the scaling laws of the LieRE generator capacity by imposing a block diagonal structure on the generator that allows us to vary the added capacity. With a head dimension of 64 LieRE adds 4032 parameters to a transformer designed for $2D$ data. While this is a small number of parameters, they lie in a critical point in the architecture, and understanding the marginal impact of this capacity can help inform computational tradeoffs.

The block diagonal generator structure results in a block-diagonal rotation matrix after the matrix exponential. The parameters for each block are learned separately. This setup allows us to vary the capacity of LieRE without modifying the rest of the model.

In the last part, we measure how much different models depend on the positional information in the image by shuffling the patches. A higher accuracy drop means the model relies more on the positions of the patches during inference.

4.2.2 3D Classification

In this section, we introduce Rotary Position Encodings for 3D data and compare LieRE-based transformers with transformers with RoPE-mixed and absolute encoding similar to the previous section [1, 11].

For the 3D experiments we examine video classification performance in the UCF101 dataset [19] and hemorrhage classification on the RSNA dataset [20]. We treat the RSNA dataset as a binary classification problem, asking the model to identify whether a 3D brain scan has a hemorrhage or not.

Again, we did not optimize any hyperparameters for the LieRE model. We additionally use Mixup described standard used augmentation method for videos [26]. The full set of hyperparameters may be found in appendix A.

5 Results

5.1 Accuracy

For 2D images, we show that the LieRE-based transformer outperforms the DeiT by 5.5% [23], RoPE adaptation in VisionLlama [3] by 3.6% and RoPE-Mixed by 2.7% on Cifar100 [11].

For 3D inputs (video and 3D medical images), we observe an accuracy improvement of LieRE-based transformer over the Absolute Position Embedding of up to 6.7 % and RoPE-based transformers by up to 2.5% in accuracy.

Table 1: 2D image classification on Cifar100 and ImageNet [13, 5], * equivalent to DeiT

Method	# params	Cifar100 Accuracy (%)	ImageNet Accuracy (%)
Absolute Position E.*	85.1M	63.9	66.1
VisionLlama RoPE	85.1M	65.8	-
RoPE-Mixed	85.1M	66.7	68.5
LieRE (ours)	85.1M	**69.4**	**68.8**

Table 2: 3D video classification on RSNA hemorrhage prediction and UCF101 dataset [19, 20], * equivalent to Vivit (spatio-temporal)

Method	# params	UCF101 Accuracy (%)	RSNA Accuracy (%)
Absolute Position E.*	88.7M	44.4	80.7
RoPE-Mixed	88.7M	48.6	81.9
LieRE (ours)	88.7M	**51.1**	**82.7**

5.2 Data efficiency

We observe that transformers based on LieRE exhibit greater data efficiency compared to leading transformer architectures for 2D images on the CIFAR-100 dataset. For instance, using only 40% of the dataset, the LieRE-based transformer outperforms all comparable methods by 4.47%. Additionally, there is a mild trend indicating that the performance gap widens as the amount of data decreases (Figure 2b).

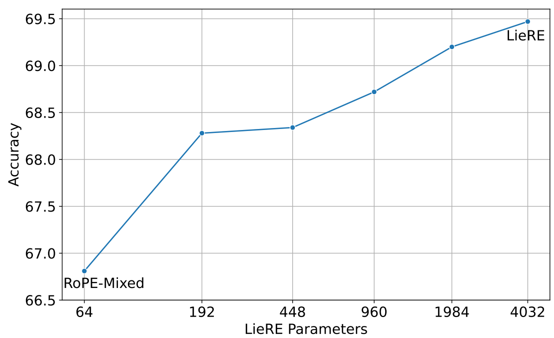
5.3 Generator Dimension Scaling Laws

LieRE adds a small amount of capacity to the model (4032 parameters in our case) but still represents the largest amount of learnable capacity around relative position encodings to date. This leads to the natural question of how helpful marginal capacity is.

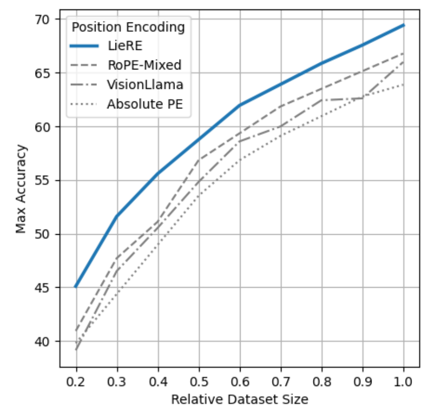
We vary capacity by enforcing a block diagonal structure on the generator. varying the block size allows us to approach "full" LieRE. Note that 2×2 blocks correspond exactly to RoPE-Mixed.

In figure 2a we evaluate accuracy versus block dimension. We observe the steepest increase at the very start, though accuracy continues to grow as the generator dimension increases.

5.4 Compute efficiency



(a) Performance scales with generator dimension (learnable parameters)



(b) Data ablation on Cifar100

Figure 2

Training transformers can necessitate substantial computational resources, which can hinder equitable access to research and development of machine learning methods. We demonstrate that the LieRE-based transformer requires 3.5 times less training time to achieve comparable performance to the Absolute Position Embedding baseline (as used in DeiT III [23]). This represents the largest reduction in training time compared to recent works such as VisionLlama and RoPE-Mixed [3, 11]. We note that this is the first training efficiency comparison of these recent methods. Figure 3 shows the amount of allowable compute reduction to achieve the same accuracy achieved by absolute position encodings (DEIT baseline) after 200 epochs. LieRE demonstrates the largest win, allowing a 3.5X reduction in training compute to achieve the same accuracy.

While all methods display better performance with more training compute, a $3.5x$ reduction allows for significantly faster experimentation and makes a fixed level of performance more accessible to those with limited access to compute resources.

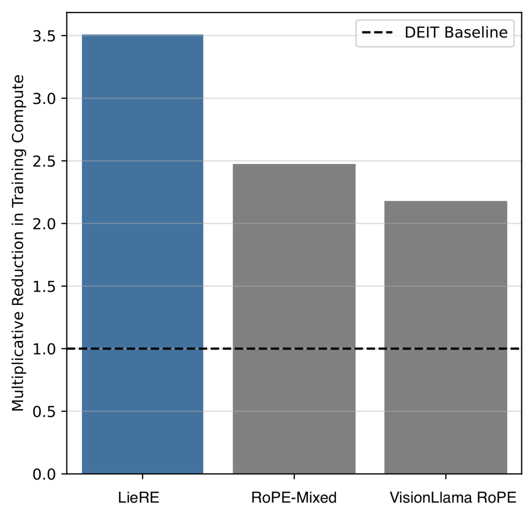


Figure 3: The LieRE spatial encoding allows the model to match the performance of absolute position encodings with substantially less training time.

5.5 Patch shuffling

Shuffling patches and frames allows us to see how much the model is able to use the positional information in its inputs. A model whose architecture does not allow/encourage the use of positional information will converge to a representation similar in spirit to a bag-of-words, where the relative locations of pixels/voxels do not matter. A greater dropoff in accuracy during shuffling is indicative that the model more heavily utilizes positional information.

We evaluate models using the decline in accuracy when evaluating on shuffled patches. We observe the most significant decline LieRE-based transformers, leading to the conclusion that LieRE encodes meaningful relative positions between tokens. The complete results are displayed in table 3 for cifar100 and table 4 for UCF101.

Table 3: Relative drop in accuracy for 2D image classification after shuffling patch order, Cifar100

Method	before shuffling ↑	after shuffling ↓	Accuracy Drop (%) ↑
Absolute Position E.*	63.9	19.6	69.3
VisionLlama RoPE	65.8	29.7	54.8
RoPE-Mixed	66.7	16.5	75.4
LieRE (ours)	**69.4**	**15.9**	**77.1**

Table 4: Accuracy for Video recognition after patch shuffling, UCF101 dataset

Method	before shuffling ↑	after shuffling ↓	Accuracy Drop (%) ↑
Absolute Position E.*	44.4	44.0	0.1
RoPE-Mixed	48.6	36.6	24.7
LieRE (ours)	**51.1**	**32.2**	**36.9**

6 Limitations

While LieRE shows promising results across multiple modalities and input dimensionalities, there are a few limitations worth noting:

1. **Compatibility with architectures that do not use attention**: Our method is specifically designed to modify the inner product, making it compatible with most attention schemes, including original attention and linear attention. However, this specificity may limit its applicability to other architectures, like convolutional neural networks, that do not rely on inner product-based attention mechanisms. Future work could explore adaptations of our method to a wider range of architectures.

2. **Limited to positions in $\mathbb{R}^n$**: The current formulation of our method is designed to encode positions in $\mathbb{R}^n$. While this is sufficient for many applications, it may not be directly applicable to tasks that require encoding poses in $SE(3)$, like robotics. Further research may be necessary to adapt our method to effectively handle such representational requirements.

Despite these limitations, we believe that our work provides much-needed insight into how to improve model performance and reduce training costs by encoding relative position information across various modalities and input dimensionalities.

7 Broader Impacts

LieRE, our proposed method for encoding positional information in attention mechanisms, has demonstrated substantial improvements in 2D and 3D image classification tasks. We are particularly excited about how LieRE can expand the applicability of RoPE-based transformers to n dimensions. This lays down the tracks to apply that same relative position within and across modalities and settings.

1. **One Backbone for All Modalities**: LieRE enhances the generalizability of attention mechanisms, making them more versatile and adaptable to a wider range of modalities. Once the input is encoded as tokens and positions, no additional changes are necessary in order to support a new modality. By providing a flexible and efficient way to encode positional information, LieRE can facilitate the application of attention mechanisms to diverse data types, such as audio, video, multi-dimensional sensor data or temporal data with diverse time intervals. This increased generalizability can lead to more effective transfer learning and cross-pollination of ideas between different research areas, accelerating progress and innovation in the field.

2. **Improving accessibility of attention-based architectures for low-data and low-compute regimes**: This is particularly valuable for applications where labeled spatial data is scarce or expensive to acquire, such as in medical imaging and robotics. By lowering the barriers to entry, LieRE can enable the application of attention mechanisms to a broader set of problems, including those in resource-constrained settings or niche domains.

3. **Enabling more efficient and sustainable AI**: The reduced training costs and improved data efficiency associated with LieRE can contribute to the development of more efficient and sustainable AI systems. By requiring fewer computational resources and less training data, LieRE can help mitigate the environmental impact of large-scale model training. This is particularly important as the field of AI continues to grow and the demand for computational resources increases.

In conclusion, LieRE has the potential to expand the generalizability of attention mechanisms, improve their accessibility for spatial data, and contribute to the development of more efficient and sustainable AI systems.

8 Conclusion

In this paper, we introduced Lie group Relative position Encodings (LieRE), a position encoding that can effectively encode relative position information for attention mechanisms across modalities and input dimensionalities. Through extensive experiments on 2D image classification (CIFAR100, ImageNet) and 3D medical image classification (RSNA brain CT hemorrhage detection), we demonstrated that LieRE achieves superior performance compared to existing positional encoding methods. Beyond improving accuracy, LieRE also exhibits data and compute efficiency. On CIFAR100, LieRE requires 3.5 times less training computed to match the performance of the baseline model with absolute position encodings. Furthermore, LieRE can outperform the baseline trained on the full dataset while using only 70% of the training data, highlighting its data efficiency. The key advantages of LieRE include its simplicity, flexibility, and ease of adaptation to new modalities. By requiring no changes to the tokenizer other than outputting positions in $\mathbb{R}^n$ and no other code changes, LieRE provides a unified and efficient approach for transformers to process and learn from various data modalities within a single architecture.

We hope that this empowers the field in building models that can understand concepts.

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A Experiment Hyperparameters

The backbone for all experiments is configured as ViT-B, with 12 layers, a hidden dimension of 768, and an intermediate dimension of 3096. We use dropout of 0.1.

A.1 2D Image Classification

The CIFAR experiments where trained on 8xL4 GPUs with 24GB of VRAM each and all took under 30 minutes to complete. The generator scaling experiment was conducted using RTX6000 GPUs. The ImageNet experiments were trained on 8xL40 GPUs and all took less than 2 days and 5 hours of runtime including time lost due to preemption and resource sharing. We use a cosine learning rate schedule with an initial learning rate of $1E-4$ and train for 200 epochs. We use an effective batch size of 512. We use a patch size of 4×4 on the original 32×32 image for Cifar100 and a patch size of 16×16 on the randomly cropped and resized 224×224 image. All vision experiments used RandAugment [4]. We use the ADAM optimizer with betas of 0.9 and 0.999 and $\epsilon = 1e-8$. The hyperparameters were tuned with RoPE-mixed and selected before conducting the LieRE trainers as to ensure a fair comparison.

A.2 3D Medical Image and Video Classifications

The 3D classification experiments were conducted on either $8 \times A100$ 40GB GPUs or $4 \times A100$ 80GB GPUs with the effective batch size held constant either by using a gradient accumulation or increasing the batch size. Similar to 2D classification, we use an initial learning rate of $1E-4$ with a cosine decay, trained for 200 epochs, and had a total batch size of 64 and a patch size of $4 \times 16 \times 16$ on the randomly cropped and resized $32 \times 224 \times 224$ video/image. We use the ADAM optimizer with betas of 0.9 and 0.999 and $\epsilon = 1e-8$. We use Mixup for all 3D experiments [22, 26].