

UnitNorm: Rethinking Normalization for Transformers in Time Series

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Abstract

Normalization techniques are crucial for enhancing Transformer models' performance and stability in time series analysis tasks, yet traditional methods like batch and layer normalization often lead to issues such as token shift, attention shift, and sparse attention. We propose UnitNorm, a novel approach that scales input vectors by their norms and modulates attention patterns, effectively circumventing these challenges. Grounded in existing normalization frameworks, UnitNorm's effectiveness is demonstrated across diverse time series analysis tasks, including forecasting, classification, and anomaly detection, via a rigorous evaluation on 6 state-of-the-art models and 10 datasets. Notably, UnitNorm shows superior performance, especially in scenarios requiring robust attention mechanisms and contextual comprehension, evidenced by significant improvements by up to a 1.46 decrease in MSE for forecasting, and a 4.89% increase in accuracy for classification. This work not only calls for a reevaluation of normalization strategies in time series Transformers but also sets a new direction for enhancing model performance and stability. The source code is available at <https://anonymous.4open.science/r/UnitNorm-5B84>.

1 Introduction

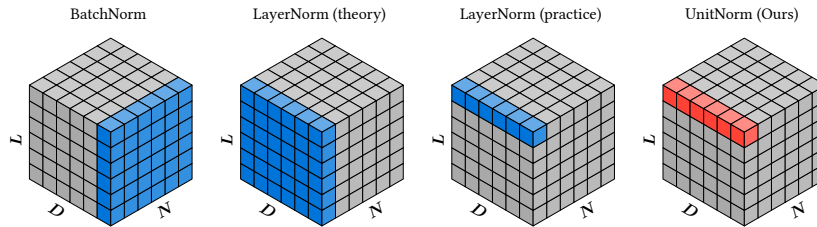


Figure 1: Scheme of different normalization methods. The input to the normalization layers is batched sequences of token vectors $\mathbf{X} \in \mathbb{R}^{N \times L \times D}$, where N is the batch size, L is the sequence length and D is the dimension of each token vector. The blue sections demonstrate a single slice of the input tensor for computing the mean μ and variance σ^2 , while the red section shows a single slice of data for computing the vector norm $\|\mathbf{x}\|$ (see Appendix C.1).

Transformers have revolutionized sequence modeling, demonstrating unparalleled efficacy across diverse fields such as natural language processing (NLP, Wolf et al. 1), computer vision (CV, Han et al. 2), and recently, time series analysis (TSA, Wen et al. 3). Central to these models is the representation of data as sequences of token vectors, denoted by $\mathbf{X} \in \mathbb{R}^{N \times L \times D}$, where N stands for batch size, L is the sequence length and D represents the dimensionality of each token. The core mechanism facilitating the Transformers’ ability to model complex dependencies is the attention mechanism. It computes a weighted sum of value vectors \mathbf{V} , capturing the sequential relationships between tokens through a scalable dot-product operation of queries \mathbf{Q} and keys \mathbf{K} [4]:

$$\text{Attention}(\mathbf{Q}, \mathbf{K}, \mathbf{V}) = \text{softmax} \left(\frac{\mathbf{Q}\mathbf{K}^\top}{\sqrt{D}} \right) \mathbf{V}, \quad (1)$$

To mitigate issues during the training process of Transformers related to vanishing or exploding gradients [5, 6], Layer Normalization (LayerNorm, LN, Ba et al. 7) plays a significant role and is therefore incorporated at each sub-layer of the architecture (Figure S1)¹. The LayerNorm operation follows the center-and-scale standardization paradigm, by first centering the means to 0 and then rescaling the variances of the input vectors to 1 [7] such that

$$\text{LN}(\mathbf{X}) = \frac{\mathbf{X} - \boldsymbol{\mu}}{\sqrt{\boldsymbol{\sigma}^2 + \varepsilon}}, \quad (2)$$

where $\boldsymbol{\mu}$ and $\boldsymbol{\sigma}$ are the mean and standard deviation of the input vector \mathbf{X} , respectively.

While LayerNorm, compared to other normalization strategies such as batch normalization [8–10], has established itself as the dominant normalization strategy in Transformers, dedicated normalization-specific research has mostly focussed on its impact on model convergence [11], its inner dynamics [10, 9] or its location [12] within the architecture. On the other hand, only few works touch upon the interaction of normalization with the attention mechanism [13] (see also Related Work Section 5.1), which poses specific challenges in TSA (see Section 2) due to the dot product in attention mechanism.

In this work, we provide a new viewpoint on these challenges by first identifying and formalizing Transformer-specific challenges of normalization techniques, highlighting three key issues. Building on these insights, we introduce a novel normalization technique, UnitNorm, designed to address these challenges effectively.

Our contributions lie in: 1) We originally identify two challenges, namely *token shift* and *attention shift*, and reassess the challenge of *sparse attention* in Transformers [14]; 2) We propose a new normalization method, UnitNorm, that can mitigate these issues by design; 3) We empirically validate the effectiveness of UnitNorm on nine datasets spanning three downstream TSA tasks.

2 Challenges in Normalization

Transformers rely on attention mechanisms to achieve remarkable performance in time series analysis tasks. However, the interplay between the attention mechanism and the applied normalization methods introduces critical challenges that have yet to be fully addressed. This paper aims to shed light on the complexities of token shift, attention shift, and sparse attention, which arise from the interaction between normalization and the attention mechanism within Transformer models. By presenting a thorough theoretical and empirical analysis, we demonstrate that these challenges are intrinsic to the conventional approaches to normalization, impacting the efficacy of the self-attention mechanism that is central to all Transformer-based architectures.

We explore the relationship between normalization and the attention mechanism by examining a simplified equivalent attention process, where the normalization layer precedes the attention computation (Zhang et al. 15, Figure S1). This perspective allows for a detailed exploration of how normalization influences the attention scores derived from the query and key vectors. For simplicity, our discussion will center on a singular instance of self-attention within the encoder layer, assuming identical query and key vectors to streamline our analysis (see Appendix C.2).

Table 1: Effect of input transformations on the softmax function output. Importance order invariant refers to whether the relative importance of the tokens is preserved. Of all possible input transformations, only the reflection transformation will definitely change the importance order of the tokens.

| Type | Function | Input | | | Output | | | Order invariant? |
|------------|--|-------|-----|----|--------|------|------|------------------|
| None | $f : x \mapsto x$ | -2 | 1 | 3 | 0.01 | 0.12 | 0.88 | |
| Stretch | $f : x \mapsto k \cdot x, k \in \mathbb{R}^+$ | -4 | 2 | 6 | 0 | 0.02 | 0.98 | ✓ |
| Translate | $f : x \mapsto x + a, a \in \mathbb{R}$ | -1 | 2 | 4 | 0.01 | 0.12 | 0.88 | ✓ |
| Jitter | $f : x \mapsto x + \varepsilon, \varepsilon \sim \mathcal{N}(0, \sigma^2)$ | -2.1 | 1.1 | 3 | 0.01 | 0.13 | 0.87 | ✓/✗ |
| Reflection | $f : x \mapsto -x$ | 2 | -1 | -3 | 0.95 | 0.05 | 0.01 | ✗ |

Table 2: Effect of normalization on the attention weight distribution based on empirical results (Figures S6 and S7). UnitNorm shows the most faithful representation of the original attention weights that are cross-validated by various metrics as described in Table S9, while center-and-scale normalization significantly alters the attention weights to an extreme extent as depicted in Figure S5.

| Normalization | Chebyshev distance ↓ | Cosine similarity ↑ | KL divergence ↓ | Entropy ↑ |
|------------------|----------------------|---------------------|-----------------|-----------|
| None (original) | / | / | / | High |
| Center-and-scale | High | Low | High | Very Low |
| UnitNorm | Low | High | Low | High |

2.1 Token shift

Previous study [16] has attributed LayerNorm’s efficacy to its center-and-scale operations: centering projects the input vectors to a hyperplane orthogonal to $\mathbf{1}$ vector, and scaling normalizes the vectors to a unit sphere to prevent any token vector being contained in the convex hull of the others. However, this can significantly alter the orientation of input vectors, especially for those that are near parallel to the hyperplane’s norm vector $\mathbf{1}$. This alteration impacts the dot product between vectors, potentially leading to sign flips (Figure 2). Such flips can severely disrupt the softmax function’s output (Table 1), altering the relative importance of tokens **in a catastrophic way that might convert a significant token into an insignificant one, or vice versa** (Table 2). This issue of significant deviations in attention weight distributions caused by token shift will be further explored in Section 2.2.

¹The LayerNorm used in Transformers, referred to as LayerNorm (practice), computes the statistics within each token rather than over the whole batch as LayerNorm (theory) does (Figure 1). In this paper, we will refer to the LayerNorm (practice) as LayerNorm if no distinction is made.

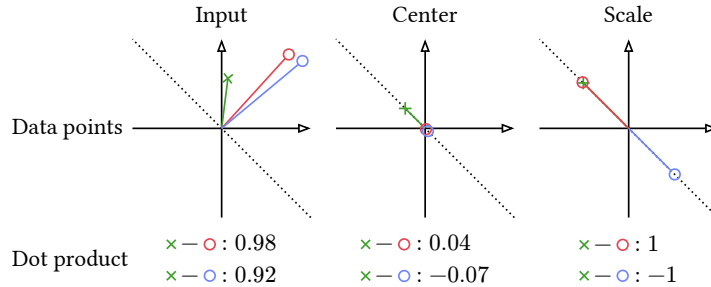


Figure 2: Case of token shift in LayerNorm. The green cross denotes a query vector, the red and blue circles denote two key vectors. The token shift happens at the centering step of normalization and causes sign flip in dot product, while the scale step will not have such an effect.

Unfortunately, the propensity for "center-and-scale" normalization to induce such undesirable sign flips in the dot product of vectors is not merely theoretical; it occurs with a high probability, as elucidated by the following theorem.

Theorem 2.1 (High probability of sign flip due to center operation). *Assume that $\mathbf{x} \sim \mathcal{N}(\boldsymbol{\mu}_x, \text{diag}(\boldsymbol{\sigma}_x^2))$, $\mathbf{y} \sim \mathcal{N}(\boldsymbol{\mu}_y, \text{diag}(\boldsymbol{\sigma}_y^2))$ are two independent token vectors, with $\boldsymbol{\mu}_x, \boldsymbol{\mu}_y, \boldsymbol{\sigma}_x, \boldsymbol{\sigma}_y \in \mathbb{R}^D$. Let $\tilde{\mathbf{x}} = \frac{\mathbf{x} - \boldsymbol{\mu}_x}{\boldsymbol{\sigma}_x}$ and $\tilde{\mathbf{y}} = \frac{\mathbf{y} - \boldsymbol{\mu}_y}{\boldsymbol{\sigma}_y}$ be the normalized vectors. If*

$$|\boldsymbol{\mu}_x^\top \boldsymbol{\mu}_y| \geq 12 \left(\sqrt{\boldsymbol{\sigma}_x^{2\top} \boldsymbol{\sigma}_y^2} + \|\boldsymbol{\sigma}_x \circ \boldsymbol{\sigma}_y\|_\infty \right) + 5 \left(\sqrt{\boldsymbol{\sigma}_y^{2\top} \boldsymbol{\mu}_x^2} + \sqrt{\boldsymbol{\sigma}_x^{2\top} \boldsymbol{\mu}_y^2} + \|\boldsymbol{\sigma}_y \circ \|\boldsymbol{\mu}_x\|_\infty + \|\boldsymbol{\sigma}_x \circ \|\boldsymbol{\mu}_y\|_\infty \right) \quad (3)$$

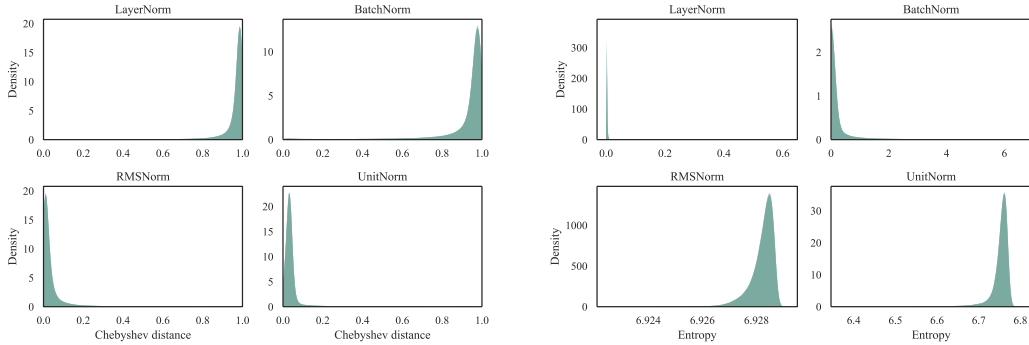
then the probability that the signs of $\mathbf{x}^\top \mathbf{y}$ and $\tilde{\mathbf{x}}^\top \tilde{\mathbf{y}}$ do not coincide is at least 40%, i.e.,

$$\Pr(\text{sgn}(\mathbf{x}^\top \mathbf{y}) \neq \text{sgn}(\tilde{\mathbf{x}}^\top \tilde{\mathbf{y}})) \geq 0.40. \quad (4)$$

Remark 2.2. Derived from the computational methodologies for the statistics of vectors \mathbf{x} and \mathbf{y} (Appendix C.1), BatchNorm posits that the mean vectors are the same so that $\boldsymbol{\mu}_x = \boldsymbol{\mu}_y = \boldsymbol{\mu}$, and similarly $\boldsymbol{\sigma}_x^2 = \boldsymbol{\sigma}_y^2 = \boldsymbol{\sigma}^2$, while LayerNorm assumes that the mean and standard deviation are shared across feature dimension: $\boldsymbol{\mu}_x = \mu_x \mathbf{1}, \boldsymbol{\mu}_y = \mu_y \mathbf{1}$ and $\boldsymbol{\sigma}_x^2 = \sigma_x^2 \mathbf{1}, \boldsymbol{\sigma}_y^2 = \sigma_y^2 \mathbf{1}$. Given these assumptions, the condition (3) outlined in Theorem 2.1 is satisfied for many token vector distributions. In fact, we show that in the setup of LayerNorm, the condition (3) allows for the quotients of token means and standard deviations, i.e., for μ_x/σ_x and μ_y/σ_y , to decay as $\Omega(D^{-1/4})$ while still implying a high sign flip probability, cf. Appendix A.

Theorem 2.1 (see Appendix B for proof) underscores the vulnerability of the "center-and-scale" normalization approach to inadvertently altering the attention mechanism's functionality. The potential for such sign flips, demonstrated with significant likelihood, poses a serious risk to the integrity of the attention scores, as it can lead to a complete reordering of the tokens' importance. We shall see that substantial presence of this issue is not only theoretical, but also empirically validated in the following section.

2.2 Attention shift



(a) Distribution of Chebyshev distance. UnitNorm and RMSNorm preserves the distribution of attention scores, while others significantly alter the distribution.

(b) Distribution of entropy. UnitNorm and RMSNorm preserves the high entropy of attention scores, while others result in a heavily unbalanced distribution.

Figure 3: Empirical statistics for attention scores after each normalization method. Results from 10 independent experiments are overlaid. $k = 1.5$ is used for UnitNorm.

Attention shift represents a critical challenge in Transformer models, directly stemming from the token shift issue. This shift perturbs the relative significance of tokens, leading to discrepancies in the attention weights generated from normalized inputs compared to those from the original, unnormalized inputs. To validate the prevalence of attention shift across normalization techniques, we conduct a study utilizing pre-trained Word2Vec embeddings [17]. Our analysis includes a comparison of batch normalization (BatchNorm, BN, Ioffe and Szegedy 8), layer normalization (LayerNorm,

LN, Ba et al. 7, Vaswani et al. 4), root mean square layer normalization (RMSNorm, RMSN, Zhang and Sennrich 18), and our proposed unit normalization (UnitNorm, UN; see Section 3).

Our investigation utilizes sequences of token vectors, $\mathbf{X} \in \mathbb{R}^{N \times L \times D}$, as inputs to the normalization layer, where N is the batch size, L is the sequence length, and D is the dimensionality of each token. The attention scores $\mathbf{A} \in \mathbb{R}^{N \times L \times L}$, given as Equation (5), are computed for 10 independent sets of 32 batches, each containing 1,024 randomly sampled embeddings from a total of 2 million. The primary goal is to assess the impact of normalization on the fidelity of attention scores \mathbf{A} and $\tilde{\mathbf{A}}$, pre- and post-normalization, using the Chebyshev distance as a metric (Table S9).

$$\mathbf{A}_{n,i} = \text{softmax} \left(\frac{\mathbf{X}_{n,i} \mathbf{X}_n^T}{\sqrt{D}} \right) \quad (5)$$

where $\mathbf{A}_{n,i} \in \mathbb{R}^L$ is the attention scores for the i -th anchor token $\mathbf{X}_{n,i}$ to the context sequence \mathbf{X}_n from the n -th batch; $\tilde{\mathbf{A}}$ is computed similarly from normalization output $\tilde{\mathbf{X}}$.

The probability density distributions of Chebyshev distances for each normalization method, depicted in Figure 3(a), reveal significant findings of the inability of maintaining faithful attention distribution of current normalization methods. For BatchNorm and LayerNorm, the Chebyshev distances predominantly span towards the maximum possible value of 1, suggesting a profound alteration in attention weights distribution by normalization. Conversely, UnitNorm and RMSNorm demonstrates a distribution concentrated around zero, indicating minimal disruption to the original attention scores.

The empirical evidence underscores a fundamental issue with current normalization practices in Transformers: they compromise the fidelity of attention scores, leading to distorted relational dynamics between tokens. This distortion challenges not only the model’s interpretability but also its ability to learn and adopt complex dependencies accurately.

2.3 Sparse attention

The challenge of sparse attention further complicates the normalization landscape in Transformer models. Traditional "center-and-scale" normalization methods often lead to an undesirable concentration of attention scores, effectively pushing the distribution towards one-hot. This is due to fact that centering removes a degree of freedom from the vectors, and only query that are tightly around the $\mathbf{1}$ vector can produce uniform attention scores [16]. This can be depicted by the entropy of the attention scores \mathbf{A}_i :

$$H(\mathbf{A}_i) = - \sum_{j=1}^L \mathbf{A}_{i,j} \log \mathbf{A}_{i,j} \quad (6)$$

A higher entropy value suggests a more uniform attention distribution, enabling models capturing periodicity in time series. Conversely, lower entropy, or a trend towards one-hot distributions, limits its attention to narrow ranges of tokens. While some studies [19, 14] in other fields have shown that Transformer models may benefit from capturing longer-range, denser connections, we will show later that such sparse attention is particularly problematic in TSA tasks and requires finer control over the attention patterns.

Analysis of normalization methods through the lens of attention score entropy (Figure 3(b)) reveals a stark contrast in their effects on model behavior. BatchNorm and LayerNorm significantly skew attention distributions towards minimal entropy. This condition not only narrows the model’s focus but may also precipitate training instability [14]. In contrast, UnitNorm and RMSNorm maintain higher entropy levels, suggesting a more balanced and contextually aware attention mechanism. Notably, the key deviation in attention entropy between UnitNorm and RMSNorm is the former’s ability to modulate the entropy pattern by adjusting the k parameter, as discussed in Section 3, while RMSNorm maintains a consistent high entropy level close to the theoretical upper bound $\log L$.

3 Methodology

To mitigate the challenges identified with traditional normalization methods, we introduce a novel approach called **unit normalization (UnitNorm, UN)**, formulated such that

$$\text{UN}(\mathbf{X}) = D^{\frac{k}{2}} \frac{\mathbf{X}}{\|\mathbf{X}\|_2}. \quad (7)$$

Diverging from the conventional center-and-scale paradigm, UnitNorm omits the center operation entirely. Similar to RMSNorm, UnitNorm focuses solely on scaling the input vectors, first normalizing the input vectors by their ℓ^2 norm. However, UnitNorm is different to RMSNorm through subsequently scaling them by a factor of $D^{\frac{k}{2}}$, where k is a hyperparameter dictating the sparsity of the resulting attention scores.

3.1 Theoretical foundation

UnitNorm is theoretically grounded as a variant of LayerNorm and RMSNorm. Specifically, when taking $k = 1$, UnitNorm is effectively acting as LayerNorm with asserted zero mean, and the RMSNorm can be seen as a special case of UnitNorm with $k = 1$.

This equivalence suggests that UnitNorm inherits the beneficial properties of LayerNorm and RMSNorm, such as mitigating gradient vanishing or exploding and stabilizing training. It maintains consistent forward pass and gradient propagation regardless of scaling in learnable parameters, while scaling down the gradient to these parameters when they are large (proved in Appendix B), thus ensuring stable training conditions:

Theorem 3.1 (UnitNorm preserves the gradient to the input and stabilize the gradient to the learnable parameters). *Given the output of an affine transformation $\mathbf{x} = \mathbf{W}\mathbf{v} + \mathbf{b}$, where \mathbf{W} and \mathbf{b} are learnable parameters. If $\mathbf{x}' = (\alpha\mathbf{W})\mathbf{v} + (\alpha\mathbf{b})$, then the output of UnitNorm is unchanged, i.e., $\tilde{\mathbf{x}}' = \tilde{\mathbf{x}}$, while the gradients to loss \mathcal{L} are given as follows:*

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{x}}'} \cdot \frac{\partial \tilde{\mathbf{x}}'}{\partial (\alpha\mathbf{W})} &= \frac{1}{\alpha} \cdot \frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{x}}} \cdot \frac{\partial \tilde{\mathbf{x}}}{\partial \mathbf{W}} = \frac{1}{\alpha} \cdot \frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{x}}} \cdot \mathbf{J}\mathbf{v}^\top \\ \frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{x}}'} \cdot \frac{\partial \tilde{\mathbf{x}}'}{\partial (\alpha\mathbf{b})} &= \frac{1}{\alpha} \cdot \frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{x}}} \cdot \frac{\partial \tilde{\mathbf{x}}}{\partial \mathbf{b}} = \frac{1}{\alpha} \cdot \frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{x}}} \cdot \mathbf{J} \\ \frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{x}}'} \cdot \frac{\partial \tilde{\mathbf{x}}'}{\partial \mathbf{v}} &= \frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{x}}} \cdot \frac{\partial \tilde{\mathbf{x}}}{\partial \mathbf{v}} = \frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{x}}} \cdot \mathbf{J}\mathbf{W}^\top \end{aligned} \quad (8)$$

where \mathbf{J} is the Jacobian matrix of $\tilde{\mathbf{x}}$ w.r.t. \mathbf{x} .

3.2 Overcoming defects

While UnitNorm shares similar learning dynamics with RMSNorm, by omitting the center operation, it preserves the directions of original input vectors, directly addressing the token and attention shift problems by maintaining the dot product's sign (Figure S3). This allows UnitNorm to serve as a drop-in replacement for LayerNorm and RMSNorm in time series Transformer architectures, requiring no structural modifications.

Additionally, UnitNorm confronts the sparse attention issue by introducing an entropy lower bound (ELB) for attention scores, modulated by the hyperparameter k (proved in Appendix B). This feature enables the control of attention patterns, from dense as uniform to sparse as one-hot, offering versatility in modeling attention dynamics:

Theorem 3.2 (UnitNorm guarantees an entropy lower bound independent of the input). *For a given set of L, D and a given k , there exists an entropy lower bound (ELB) of the attention scores, i.e.*

$$\text{ELB}(k; L, D) = \log(L - 1 + e^d) - \frac{de^d}{L - 1 + e^d}, \quad (9)$$

where $d = 2D^{k-\frac{1}{2}}$.

Corollary 3.3 (The ELB of UnitNorm can be any possible value by modulating k). *The ELB is a monotonically decreasing function of k for a given L, D . Furthermore, it is bounded that $\forall k$:*

$$0 < \text{ELB}(k; L, D) < \log L \quad (10)$$

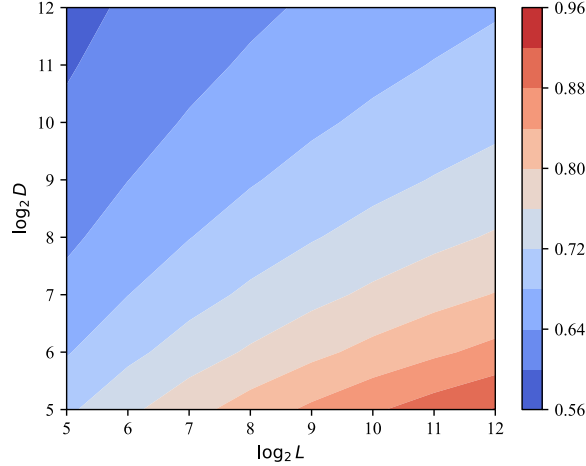


Figure 4: Landscape of k_{50} for different L, D . The k_{50} is the value of k that achieves an ELB of half of the theoretical maximum $\log L$ for a given L, D pair. The landscape of k_{50} is rather smooth and insensitive to the sequence length L , indicating UnitNorm with fixed k can be applied to sequences with variable length without significant change in the attention pattern.

The adaptability of UnitNorm is further exemplified by its applicability across variable sequence lengths, with the entropy lower bound’s sensitivity to k remaining relatively consistent irrespective of sequence length (Figure S4), along with the smooth landscape of k_{50} , the value of k that achieves an ELB of $\frac{1}{2} \log L$ for a given L, D pair (Figure 4), particularly with larger D . This property, combined with the option of setting k as a learnable parameter, empowers the model to dynamically adjust its attention pattern, optimizing performance across different tasks and data sets.

4 Experiments

In our experimental evaluation, UnitNorm is rigorously tested across a spectrum of TSA tasks to illustrate its theoretical advantages in practical applications, including long term forecasting (ETTh1, ETTh2, ECL, Exchange), classification (FaceDetection, Heartbeat, PEMS-SF, UWaveGestureLibrary) and anomaly detection (MSL). We integrate UnitNorm into various Transformer models, namely Crossformer [20], FEDformer [21], Informer [22], PatchTST [23] and the vanilla Transformer [4], all with same set of hyperparameter as described in [24]. For comparison, we also include BatchNorm, LayerNorm, RMSNorm and various settings of UnitNorm (see figure legends). By doing so, we aim to demonstrate its superior ability to address normalization-related challenges, enhancing model performance in these tasks. Detailed experimental settings and full results are provided in Tables S2 to S4 and S6 to S8. Below, we outline the significance of these tasks and the specific benefits UnitNorm brings.

Long-term forecasting: Long-term forecasting represents a significant challenge for Transformer models, primarily due to the difficulty in maintaining periodic pattern recognition over extended sequences [25]. The conventional normalization methods often exacerbate the sparse attention problem, hindering the model’s capability to capture periodicity. In contrast, UnitNorm demonstrates exceptional performance in mitigating this issue, as indicated by its superior rank over longer prediction horizon and slower increase in prediction error across various datasets (Figure 5). With a maximum increase of 1.46/0.45 in MSE/MAE on ETTh2, and 1.27/0.36 in MSE/MAE on Exchange at the longest prediction horizon, it substantiates UnitNorm’s ability to preserve the attention mechanism’s effectiveness, even with increasing prediction horizons, due to its ability to maintain a balanced attention distribution and omission of token shift and attention shift disturbances.

Classification: In classification tasks, the key challenge lies in effectively capturing long-range dependencies within sequences [26], a task at which Transformers excel. However, the efficacy of this capability can be significantly impacted by the choice of normalization method. UnitNorm, with its unique approach to normalization, has been shown to enhance model performance across multiple datasets, outperforming traditional methods in 3 out of 4 datasets on average (Figure S8), with a significant increase in accuracy of up to 4.90% on UWaveGestureLibrary, 1.95% on Heartbeat and

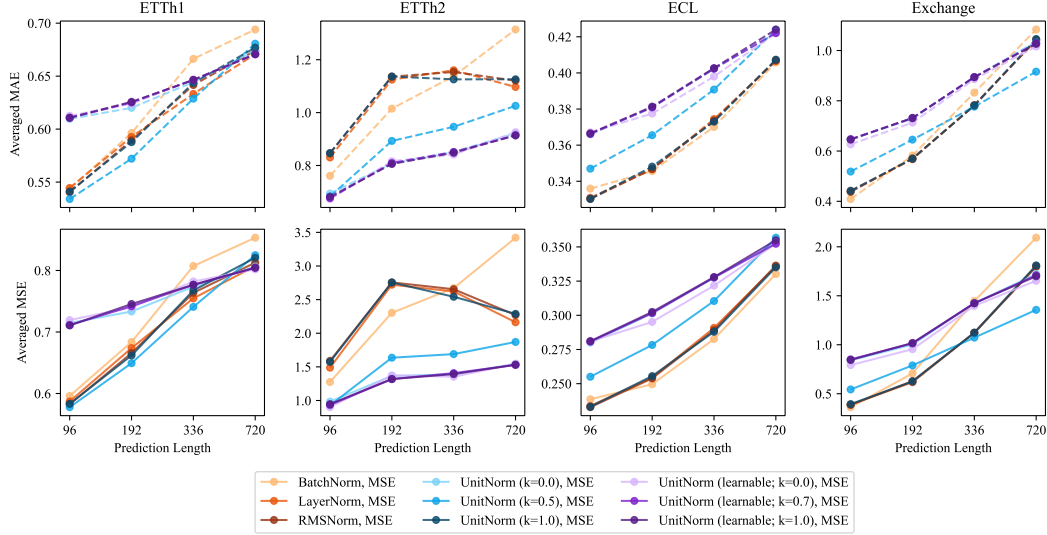


Figure 5: Average rank of normalization methods on the long-term forecasting tasks. X-axis: number of tokens to forecast, Y-axis: average rank over models. Ranks are computed based on the MAE or MSE of each model on each task with different normalization methods (lower is better). UnitNorm and UnitNorm (learnable) achieve better results with the increase of prediction horizon, and have a slower increase in prediction error compared to other normalization methods.

0.48% on FaceDetection. This underscores the versatility of UnitNorm in adapting to varied datasets, offering improved accuracy by enabling a more robust, contextually aware attention mechanism.

Anomaly detection: Anomaly detection in time series data demands robust model sensitivity to subtle deviations [27, 28], a requirement often compromised by normalization-induced shifts in attention. The token and attention shift problems, in particular, pose significant challenges in learning stable representations. UnitNorm addresses these challenges head-on, providing a more stable foundation for anomaly detection models to operate on, therefore gaining a maximum of 7.32% in recall, 5.58% in F-score, and 2.81% in precision. Its effectiveness is dominant in all accuracy, recall, precision, and F-score metrics (Figure S9), showcasing its capacity to facilitate more accurate and reliable time series modeling for anomaly detection.

5 Discussion

This study introduces UnitNorm, a normalization method tailored to Transformers that addresses the inherent limitations of currently prevalent normalization techniques. Here, we reflect on the broader implications of our findings and chart potential avenues for future research.

5.1 Related work

The development of effective normalization techniques is crucial in the optimization of neural network training, particularly for Transformer models [11]. This section reviews notable contributions in this field, providing a context for our proposed UnitNorm method.

The quest for effective normalization in neural networks, particularly Transformers, is ongoing, with significant strides made in understanding and optimizing these models’ training dynamics [11]. However, we can see that UnitNorm is fundamentally different from existing research directions, and provides a novel perspective on the role of normalization in Transformer models.

Normalization layer placement: The discourse around normalization in Transformer models has predominantly revolved around its placement: Post-Layer Normalization (Post-LN) versus Pre-Layer Normalization (Pre-LN), highlighting its impact on training stability and gradient flow [12]. Our approach with UnitNorm shifts focus from placement to the essence of normalization itself,

emphasizing the importance of preserving token vector direction being crucial for the attention mechanism, a perspective that can be applied to both Post-LN and Pre-LN Transformers.

Normalization layer design for Transformers: Following RMSNorm [18], UnitNorm eliminates the center operation in normalization and alleviate token shift and attention shift problem, while owning a fundamental departure by introducing a hyperparameter k to modulate the sparsity of attention scores. This design choice is unique to aid capturing periodicity in time series data.

Normalization on model weight: Another parallel can be drawn with Weight Normalization [29], which, despite its computational similarity to UnitNorm, applies to model parameters rather than inputs. Weight Normalization also focused on re-parameterizing for training acceleration, and thus still requires a modified BatchNorm for normalization on layer data. This distinction underscores UnitNorm’s unique approach to addressing the input-specific challenges in Transformers, diverging from methods that primarily focused on parameter optimization.

5.2 Adopting UnitNorm in Transformer models

UnitNorm invites reconsideration of standard normalization practices in Transformers, suggesting alternatives that might enhance model performance and stability. Its simplicity and versatility suggest it could be readily adopted across various Transformer applications. The broader impact of UnitNorm lies in its potential to improve the applicability and efficiency of Transformers in fields where precision and model stability are paramount. By addressing specific normalization-related challenges, UnitNorm can make Transformers more suitable for tasks with complex sequential relationships.

6 Limitations

While UnitNorm represents a significant advancement in normalization techniques for Transformers, several areas still warrant further investigation:

- **Dynamic and Adaptive Normalization:** Investigating UnitNorm’s adaptability, particularly the dynamic adjustment of the hyperparameter k , could lead to performance optimizations tailored to specific tasks.
- **Broader Application Scope:** Extending the application of UnitNorm beyond Transformers to other neural network architectures could provide valuable insights into the fundamental principles of normalization across deep learning models.
- **Cross Domain Validation:** Applying UnitNorm across diverse domains and challenging datasets beyond TSA, e.g., NLP [30, 31] and CV [32], will further elucidate its effectiveness and generalizability, providing insights into its broad utility in deep learning.
- **Problem characterization:** Understanding how and what certain dataset characteristics influence the efficacy of normalization methods, including quantitatively assess the presence of token shift, attention shift, and sparse attention in the dynamic interplay of attention mechanisms and normalization during training, can guide the community in selecting appropriate techniques for varied deep learning challenges.

Much as UnitNorm marks a promising advancement in normalization for Transformers, its exploration is far from complete. The limitations identified herein not only highlight the need for further empirical validation across domains but also the potential for refining and extending the methodology to accommodate a wider array of neural network architectures and applications.

7 Conclusion

Through the introduction of UnitNorm, this study challenges prevailing norms around normalization in Transformer models for TSA tasks, underscoring the importance of a tailored approach to normalization. UnitNorm’s innovative strategy, eschewing the conventional center operation, directly addresses the critical issues of token shift, attention shift that we have identified, along with sparse attention, which have been overlooked in traditional normalization practices.

Our contribution extends beyond the theoretical introduction of UnitNorm; it includes empirical evidence showcasing its efficacy across various tasks, setting a new precedent for normalization techniques within the Transformer architecture. By facilitating a more stable and faithful represen-

tation learning, UnitNorm paves the way for enhanced performance and broader applicability of Transformer models in complex sequential data analysis.

While there are also many potential ethical consequences of our work, given the theoretical nature of this work, a detailed discussion on ethical impacts falls beyond its scope. Future endeavors that leverage UnitNorm in application-specific contexts should carefully assess these considerations.

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A Dimension Dependence of Sign-Flip Probability

We recall that Theorem 2.1 provided a condition for token vector means and variances, condition (3), to imply that the sign of the token dot product $\mathbf{x}^\top \mathbf{y}$ is flipped by center-and-scale standardization as in LayerNorm [7].

In this section, we elucidate the dimension dependence of the required relationship between token means and standard deviations implied by this condition in the case of shared means and standard deviations across feature dimensions, such as implicitly assumed by LayerNorm.

Corollary A.1. *Assume that the mean and variance vectors of independent token vectors \mathbf{x} and \mathbf{y} satisfy $\boldsymbol{\mu}_x = \mu_x \mathbf{1}$, $\boldsymbol{\mu}_y = \mu_y \mathbf{1}$ and $\boldsymbol{\sigma}_x^2 = \sigma_x^2 \mathbf{1}$, $\boldsymbol{\sigma}_y^2 = \sigma_y^2 \mathbf{1}$. Then the mean-variance condition (3) of Theorem 2.1 is satisfied for all $L \geq 77$ if*

$$\frac{\mu_x}{\sigma_x} \geq \frac{6}{D^{1/4}} \quad \text{and} \quad \frac{\mu_y}{\sigma_y} \geq \frac{6}{D^{1/4}}, \quad (11)$$

Furthermore, if additionally the independent token vectors are distributed as $\mathbf{x} \sim \mathcal{N}(\boldsymbol{\mu}_x, \text{diag}(\boldsymbol{\sigma}_x^2))$, $\mathbf{y} \sim \mathcal{N}(\boldsymbol{\mu}_y, \text{diag}(\boldsymbol{\sigma}_y^2))$, then the dot product $\tilde{\mathbf{x}}^\top \tilde{\mathbf{y}}$ of normalized vectors $\tilde{\mathbf{x}} = \frac{\mathbf{x} - \boldsymbol{\mu}_x}{\boldsymbol{\sigma}_x}$ and $\tilde{\mathbf{y}} = \frac{\mathbf{y} - \boldsymbol{\mu}_y}{\boldsymbol{\sigma}_y}$ attains a sign flip with respect to the original inner products $\mathbf{x}^\top \mathbf{y}$ with probability of at least 40%.

Corollary A.1 implies that for high-dimensional token vectors with $D \gg 1$, it might become easier to satisfy (11) given an empirical token distribution, which means that sign flips of dot products after LayerNorm-style normalization might become even more prevalent in that case.

Proof of Corollary A.1. For the case of $\boldsymbol{\mu}_x = \mu_x \mathbf{1}$, $\boldsymbol{\mu}_y = \mu_y \mathbf{1}$ and $\boldsymbol{\sigma}_x^2 = \sigma_x^2 \mathbf{1}$, $\boldsymbol{\sigma}_y^2 = \sigma_y^2 \mathbf{1}$, it follows that

$$\begin{aligned} & 12 \left(\sqrt{\boldsymbol{\sigma}_x^{2\top} \boldsymbol{\sigma}_y^2} + \|\boldsymbol{\sigma}_x \circ \boldsymbol{\sigma}_y\|_\infty \right) + 5 \left(\sqrt{\boldsymbol{\sigma}_y^{2\top} \boldsymbol{\mu}_x^2} + \sqrt{\boldsymbol{\sigma}_x^{2\top} \boldsymbol{\mu}_y^2} + \|\boldsymbol{\sigma}_y \circ \boldsymbol{\mu}_x\|_\infty + \|\boldsymbol{\sigma}_x \circ \boldsymbol{\mu}_y\|_\infty \right) \\ &= 12 \left(\sqrt{D \sigma_x^2 \sigma_y^2} + \sigma_x \sigma_y \right) + 5 \left(\sqrt{D \sigma_y^2 \mu_x^2} + \sqrt{D \sigma_x^2 \mu_y^2} + \sigma_y |\mu_x| + \sigma_x |\mu_y| \right) \\ &\leq 12 \left(\sqrt{D \frac{D \mu_x^2 \mu_y^2}{36^2}} + \frac{D^{1/4} \mu_x}{6} \frac{D^{1/4} \mu_y}{6} \right) \\ &\quad + 5 \left(\sqrt{D \frac{D^{1/2} \mu_y^2}{36} \mu_x^2} + \sqrt{D \frac{D^{1/2} \mu_x^2}{36} \mu_y^2} + \frac{D^{1/4} \mu_y}{6} |\mu_x| + \frac{D^{1/4} \mu_x}{6} |\mu_y| \right) \\ &= 12 \left(D \frac{\mu_x \mu_y}{36} + D^{1/2} \frac{\mu_x \mu_y}{36} \right) + \frac{5}{6} \left(\sqrt{D D^{1/2} \mu_y^2 \mu_x^2} + \sqrt{D D^{1/2} \mu_x^2 \mu_y^2} + D^{1/4} \mu_y |\mu_x| + D^{1/4} \mu_x |\mu_y| \right) \\ &= \mu_x \mu_y \left(\frac{1}{3} D + \frac{1}{3} D^{1/2} + \frac{5}{3} (D^{3/4} + D^{1/4}) \right) \leq D \mu_x \mu_y = |\boldsymbol{\mu}_x^\top \boldsymbol{\mu}_y|. \end{aligned}$$

Here, we used in the first inequality the assumption Equation (11) and the fact that $\frac{1}{3} D^{1/2} + \frac{5}{3} (D^{3/4} + D^{1/4}) \leq \frac{2}{3} D$ for $D \geq 77$ in the last inequality. The last assertion of the theorem then follows by application of Theorem 2.1. \square

B Proofs

In this section, we detail the proofs of the theoretical results of this paper. In particular, we present the proofs of Theorem 2.1, Theorem 3.1, Theorem 3.2, Corollary 3.3, as well as of auxiliary lemmas.

B.1 Proof of Theorem 2.1

Proof of Theorem 2.1. Let $\mathbf{x} \sim \mathcal{N}(\boldsymbol{\mu}_x, \text{diag}(\boldsymbol{\sigma}_x^2))$ and $\mathbf{y} \sim \mathcal{N}(\boldsymbol{\mu}_y, \text{diag}(\boldsymbol{\sigma}_y^2))$ be independent, and write $\mathbf{x} = (X_1, \dots, X_D)$ and $\mathbf{y} = (Y_1, \dots, Y_D)$, respectively.

then we can compute the expectation $\mathbb{E} [\mathbf{x}^\top \mathbf{y}]$ of the dot product of \mathbf{x} and \mathbf{y} as

$$\begin{aligned}\mathbb{E} [\mathbf{x}^\top \mathbf{y}] &= \mathbb{E} \left[\sum_{i=1}^D X_i Y_i \right] \\ &= \sum_{i=1}^D \mathbb{E} [X_i Y_i] \\ &= \sum_{i=1}^D \mathbb{E} [X_i] \mathbb{E} [Y_i] \\ &= \sum_{i=1}^D (\boldsymbol{\mu}_x)_i (\boldsymbol{\mu}_y)_i \\ &= \boldsymbol{\mu}_x^\top \boldsymbol{\mu}_y.\end{aligned}$$

$$\begin{aligned}\text{Var} (\mathbf{x}^\top \mathbf{y}) &= \mathbb{E} \left[(\mathbf{x}^\top \mathbf{y})^2 \right] - (\mathbb{E} [\mathbf{x}^\top \mathbf{y}])^2 \\ &= \mathbb{E} \left[\left(\sum_{i=1}^D X_i Y_i \right)^2 \right] - (\boldsymbol{\mu}_x^\top \boldsymbol{\mu}_y)^2 \\ &= \sum_{i,j=1}^D \mathbb{E} [X_i Y_i X_j Y_j] - (\boldsymbol{\mu}_x^\top \boldsymbol{\mu}_y)^2 \\ &= \sum_{i,j=1}^D \mathbb{E} [X_i X_j] \mathbb{E} [Y_i Y_j] - (\boldsymbol{\mu}_x^\top \boldsymbol{\mu}_y)^2\end{aligned}\tag{12}$$

By definition of covariance, we have $\boldsymbol{\sigma}_x = \mathbb{E} [\mathbf{x} \mathbf{x}^\top] - \boldsymbol{\mu}_x \boldsymbol{\mu}_x^\top$, and here $\boldsymbol{\sigma}_x = \text{diag}(\boldsymbol{\sigma}_x^2)$, then Equation (12) can be simplified as follows:

$$\begin{aligned}\text{Var} (\mathbf{x}^\top \mathbf{y}) &= \sum_{i,j=1}^D (\boldsymbol{\sigma}_x + \boldsymbol{\mu}_x \boldsymbol{\mu}_x^\top)_{ij} (\boldsymbol{\sigma}_y + \boldsymbol{\mu}_y \boldsymbol{\mu}_y^\top)_{ij} - (\boldsymbol{\mu}_x^\top \boldsymbol{\mu}_y)^2 \\ &= \langle \boldsymbol{\sigma}_x, \boldsymbol{\sigma}_y \rangle_F + \langle \boldsymbol{\mu}_x \boldsymbol{\mu}_x^\top, \boldsymbol{\sigma}_y \rangle_F + \langle \boldsymbol{\sigma}_x, \boldsymbol{\mu}_y \boldsymbol{\mu}_y^\top \rangle_F + \langle \boldsymbol{\mu}_x \boldsymbol{\mu}_x^\top, \boldsymbol{\mu}_y \boldsymbol{\mu}_y^\top \rangle_F - (\boldsymbol{\mu}_x^\top \boldsymbol{\mu}_y)^2 \\ &= (\boldsymbol{\sigma}_x^2)^\top (\boldsymbol{\sigma}_y^2) + (\boldsymbol{\sigma}_y^2)^\top (\boldsymbol{\mu}_x^2) + (\boldsymbol{\sigma}_x^2)^\top (\boldsymbol{\mu}_y^2)\end{aligned}\tag{13}$$

where $\langle \cdot, \cdot \rangle_F$ is the Frobenius inner product.

Consider now the normalized random vectors $\tilde{\mathbf{x}} = \frac{\mathbf{x} - \boldsymbol{\mu}_x}{\boldsymbol{\sigma}_x}$ and $\tilde{\mathbf{y}} = \frac{\mathbf{y} - \boldsymbol{\mu}_y}{\boldsymbol{\sigma}_y}$. Due to the Gaussianity assumption on \mathbf{x} and \mathbf{y} , it follows that the normalized vectors are also Gaussian, and in particular, are distributed as $\tilde{\mathbf{x}}, \tilde{\mathbf{y}} \sim \mathcal{N}(\mathbf{0}, \mathbb{I})$. Plugging the respective mean and variance values into the formulas for the expectation and variance for dot products above, we obtain that

$$\mathbb{E} [\tilde{\mathbf{x}}^\top \tilde{\mathbf{y}}] = 0 \quad \text{and} \quad \text{Var} (\tilde{\mathbf{x}}^\top \tilde{\mathbf{y}}) = 1\tag{14}$$

As $\tilde{\mathbf{x}}^\top \tilde{\mathbf{y}}$ is a symmetric random variable, it follows that

$$\Pr (\tilde{\mathbf{x}}^\top \tilde{\mathbf{y}}) = 0.5.\tag{15}$$

Next, due to the definition of the random vectors \mathbf{x} and \mathbf{y} , it holds that $\mathbf{x}^\top \mathbf{y} = \sum_{i=1}^D X_i Y_i$, where $X_i \sim \mathcal{N}((\boldsymbol{\mu}_x)_i, (\boldsymbol{\sigma}_x)_i^2)$ and $Y_i \sim \mathcal{N}((\boldsymbol{\mu}_y)_i, (\boldsymbol{\sigma}_y)_i^2)$ are independent normal random variables. Going forward, we will use the ψ_1 -Orlicz norm

$$\|X\|_{\psi_1} := \inf \{t > 0 : \mathbb{E}[\exp(|X|/t)] \leq 2\},\tag{16}$$

cf. Definition 2.7.5 of [33]. We call a random variable for which $\|\cdot\|_{\psi_1}$ is finite sub-exponential, following, e.g., [33].

Define now $Z_i := X_i Y_i - (\boldsymbol{\mu}_x)_i (\boldsymbol{\mu}_y)_i$. We observe that

$$Z_i = X_i Y_i - (\boldsymbol{\mu}_x)_i (\boldsymbol{\mu}_y)_i = X_i (Y_i - (\boldsymbol{\mu}_y)_i) + (X_i - (\boldsymbol{\mu}_x)_i) (\boldsymbol{\mu}_y)_i = Z_i^{(1)} + Z_i^{(2)}$$

with $Z_i^{(1)} := X_i (Y_i - (\boldsymbol{\mu}_y)_i)$ and $Z_i^{(2)} := (X_i - (\boldsymbol{\mu}_x)_i) (\boldsymbol{\mu}_y)_i$. To bound the ψ_1 -norm of Z_i , we bound this norm for $Z_i^{(1)}$ and $Z_i^{(2)}$ separately.

Indeed, due to Lemma 2.7.7 of [33], it holds that

$$\|Z_i^{(1)}\|_{\psi_1} \leq \|X_i\|_{\psi_2} \|Y_i - (\boldsymbol{\mu}_y)_i\|_{\psi_2},$$

where

$$\|X\|_{\psi_2} := \inf\{t > 0 : \mathbb{E}[\exp(X^2/t^2)] \leq 2\}, \quad (17)$$

is the ψ_2 -Orlicz norm [33] characterizing sub-Gaussian random variables X . From Lemma B.2, it follows therefore that

$$\|Z_i^{(1)}\|_{\psi_1} \leq \max \left(2(\boldsymbol{\sigma}_x)_i, \sqrt{\frac{(\boldsymbol{\mu}_x)_i^2}{\log 2} + (\boldsymbol{\sigma}_x)_i^2} \right) \sqrt{\frac{8}{3}} (\boldsymbol{\sigma}_y)_i.$$

For the second part, since $\|\cdot\|_{\psi_2}$ is a norm, we estimate that

$$\|Z_i^{(2)}\|_{\psi_1} \leq \|X_i - (\boldsymbol{\mu}_x)_i\|_{\psi_2} \|(\boldsymbol{\mu}_y)_i\|_{\psi_2} \leq \sqrt{\frac{8}{3}} (\boldsymbol{\sigma}_x)_i \|(\boldsymbol{\mu}_y)_i\|_{\psi_2} \leq \sqrt{\frac{8}{3}} (\boldsymbol{\sigma}_x)_i \frac{|(\boldsymbol{\mu}_y)_i|}{\sqrt{\log 2}},$$

where we used again Lemma 2.7.7 and (2.17) of [33] in the first and last inequality, respectively, and Lemma B.2 in the second inequality.

From this, it follows that

$$\begin{aligned} \|Z_i\|_{\psi_1} &\leq \|Z_i^{(1)}\|_{\psi_1} + \|Z_i^{(2)}\|_{\psi_1} \leq \max \left(2(\boldsymbol{\sigma}_x)_i, \sqrt{\frac{(\boldsymbol{\mu}_x)_i^2}{\log 2} + (\boldsymbol{\sigma}_x)_i^2} \right) \sqrt{\frac{8}{3}} (\boldsymbol{\sigma}_y)_i + \sqrt{\frac{8}{3}} (\boldsymbol{\sigma}_x)_i \frac{|(\boldsymbol{\mu}_y)_i|}{\sqrt{\log 2}} \\ &\leq \left(2(\boldsymbol{\sigma}_x)_i + \sqrt{\frac{(\boldsymbol{\mu}_x)_i^2}{\log 2} + (\boldsymbol{\sigma}_x)_i^2} \right) \sqrt{\frac{8}{3}} (\boldsymbol{\sigma}_y)_i + \sqrt{\frac{8}{3}} (\boldsymbol{\sigma}_x)_i \frac{|(\boldsymbol{\mu}_y)_i|}{\sqrt{\log 2}} \\ &\leq 2\sqrt{6} (\boldsymbol{\sigma}_x)_i (\boldsymbol{\sigma}_y)_i + \sqrt{\frac{8}{3}} (\boldsymbol{\sigma}_y)_i \frac{|(\boldsymbol{\mu}_x)_i|}{\sqrt{\log 2}} + \sqrt{\frac{8}{3}} (\boldsymbol{\sigma}_x)_i \frac{|(\boldsymbol{\mu}_y)_i|}{\sqrt{\log 2}}, \end{aligned} \quad (18)$$

using that $\sqrt{a^2 + b^2} \leq a + b$ for any non-negative $a, b \geq 0$ in the last inequality. We next establish a lower bound on the probability of a sign flip through normalization, i.e., for $\Pr(\text{sgn}(\mathbf{x}^\top \mathbf{y}) \neq \text{sgn}(\tilde{\mathbf{x}}^\top \tilde{\mathbf{y}}))$. Assuming without loss of generality that $|\boldsymbol{\mu}_x^\top \boldsymbol{\mu}_y| = \boldsymbol{\mu}_x^\top \boldsymbol{\mu}_y$, we observe that

$$\begin{aligned} \Pr(\text{sgn}(\mathbf{x}^\top \mathbf{y}) \neq \text{sgn}(\tilde{\mathbf{x}}^\top \tilde{\mathbf{y}})) &= \Pr((\mathbf{x}^\top \mathbf{y} > 0) \wedge (\tilde{\mathbf{x}}^\top \tilde{\mathbf{y}} < 0)) + \Pr((\mathbf{x}^\top \mathbf{y} < 0) \wedge (\tilde{\mathbf{x}}^\top \tilde{\mathbf{y}} > 0)) \\ &\geq \Pr((\mathbf{x}^\top \mathbf{y} > 0) \wedge (\tilde{\mathbf{x}}^\top \tilde{\mathbf{y}} < 0)). \end{aligned}$$

Furthermore, since the distribution of the normalized vectors $\tilde{\mathbf{x}}$ and $\tilde{\mathbf{y}}$ is symmetric, the same holds true for the dot product $\tilde{\mathbf{x}}^\top \tilde{\mathbf{y}}$, which implies that

$$\begin{aligned} \Pr((\mathbf{x}^\top \mathbf{y} > 0) \wedge (\tilde{\mathbf{x}}^\top \tilde{\mathbf{y}} < 0)) &= 1 - \Pr((\mathbf{x}^\top \mathbf{y} \leq 0) \vee (\tilde{\mathbf{x}}^\top \tilde{\mathbf{y}} \geq 0)) \geq 1 - \Pr(\mathbf{x}^\top \mathbf{y} \leq 0) - \Pr(\tilde{\mathbf{x}}^\top \tilde{\mathbf{y}} \geq 0) \\ &\geq 1 - 0.5 - \Pr(\mathbf{x}^\top \mathbf{y} \leq 0) = 0.5 - \Pr(\mathbf{x}^\top \mathbf{y} \leq 0). \end{aligned}$$

It remains to show that

$$\Pr(\mathbf{x}^\top \mathbf{y} \leq 0) \leq 0.1. \quad (19)$$

To establish this, we see that

$$\begin{aligned} \Pr(\mathbf{x}^\top \mathbf{y} \leq 0) &= \Pr(\mathbf{x}^\top \mathbf{y} - \mathbb{E}[\mathbf{x}^\top \mathbf{y}] \leq -\mathbb{E}[\mathbf{x}^\top \mathbf{y}]) = \Pr(\mathbf{x}^\top \mathbf{y} - \boldsymbol{\mu}_x^\top \boldsymbol{\mu}_y \leq -\boldsymbol{\mu}_x^\top \boldsymbol{\mu}_y) \\ &= \Pr\left(\sum_{i=1}^D Z_i \leq -\boldsymbol{\mu}_x^\top \boldsymbol{\mu}_y\right) \end{aligned}$$

with the random variables Z_i defined above. Using the triangle inequality of the ℓ_2 -norm, it follows from (18) that

$$\sqrt{\sum_{i=1}^D \|Z_i\|_{\psi_1}^2} \leq 2\sqrt{6}\sqrt{(\boldsymbol{\sigma}_x^2)^\top \boldsymbol{\sigma}_y^2} + \sqrt{\frac{8}{3\log 2}} \left(\sqrt{(\boldsymbol{\sigma}_y^2)^\top \boldsymbol{\mu}_x^2} + \sqrt{(\boldsymbol{\sigma}_x^2)^\top \boldsymbol{\mu}_y^2} \right)$$

and that

$$\max_{i=1}^D \|Z_i\|_{\psi_1} \leq 2\sqrt{6}\|\boldsymbol{\sigma}_x \circ \boldsymbol{\sigma}_y\|_\infty + \sqrt{\frac{8}{3\log 2}} (\|\boldsymbol{\sigma}_y \circ |(\boldsymbol{\mu}_x)|\|_\infty + \|\boldsymbol{\sigma}_x \circ |(\boldsymbol{\mu}_y)|\|_\infty),$$

which implies that

$$\begin{aligned} & \sqrt{2 \sum_{i=1}^D \|Z_i\|_{\psi_1}^2} \sqrt{\log(10)} + \max_{i=1}^D \|Z_i\|_{\psi_1} \log(10) \\ & \leq 4\sqrt{3\log(10)} \sqrt{(\boldsymbol{\sigma}_x^2)^\top \boldsymbol{\sigma}_y^2} + \frac{4\sqrt{\log(10)}}{\sqrt{3\log(2)}} \left(\sqrt{(\boldsymbol{\sigma}_y^2)^\top \boldsymbol{\mu}_x^2} + \sqrt{(\boldsymbol{\sigma}_x^2)^\top \boldsymbol{\mu}_y^2} \right) \\ & \quad + 2\sqrt{6}\log(10)\|\boldsymbol{\sigma}_x \circ \boldsymbol{\sigma}_y\|_\infty + \sqrt{\frac{8}{3\log 2}} \log(10) (\|\boldsymbol{\sigma}_y \circ |(\boldsymbol{\mu}_x)|\|_\infty + \|\boldsymbol{\sigma}_x \circ |(\boldsymbol{\mu}_y)|\|_\infty) \\ & \leq 12 \left(\sqrt{(\boldsymbol{\sigma}_x^2)^\top \boldsymbol{\sigma}_y^2} + \|\boldsymbol{\sigma}_x \circ \boldsymbol{\sigma}_y\|_\infty \right) + 5 \left(\sqrt{(\boldsymbol{\sigma}_y^2)^\top \boldsymbol{\mu}_x^2} + \sqrt{(\boldsymbol{\sigma}_x^2)^\top \boldsymbol{\mu}_y^2} + \|\boldsymbol{\sigma}_y \circ |(\boldsymbol{\mu}_x)|\|_\infty + \|\boldsymbol{\sigma}_x \circ |(\boldsymbol{\mu}_y)|\|_\infty \right) \\ & \leq |\boldsymbol{\mu}_x^\top \boldsymbol{\mu}_y|, \end{aligned}$$

using the assumption (3) in the last inequality. With this inequality, we can use the fact that the Z_i are independent mean-zero sub-exponential random variables and Bernstein's inequality as stated in Lemma B.1 to conclude that

$$\begin{aligned} \Pr \left(\sum_{i=1}^D Z_i \leq -\boldsymbol{\mu}_x^\top \boldsymbol{\mu}_y \right) & \leq \Pr \left(\sum_{i=1}^D Z_i \leq - \left(\sqrt{2 \sum_{i=1}^D \|Z_i\|_{\psi_1}^2} \sqrt{\log(10)} + \max_{i=1}^D \|Z_i\|_{\psi_1} \log(10) \right) \right) \\ & \leq \exp(-\log(10)) = 0.1. \end{aligned}$$

This establishes (19), which concludes the proof. \square

Lemma B.1 (Bernstein's Inequality, cf. Lemma 5.1 of [34]). *Let Z_1, \dots, Z_D be independent mean-zero sub-exponential random variables. Then for every $t \geq 0$,*

$$\Pr \left(\sum_{i=1}^D Z_i \leq - \left(\sqrt{2 \sum_{i=1}^D \|Z_i\|_{\psi_1}^2} \sqrt{t} + \max_{i=1}^D \|Z_i\|_{\psi_1} t \right) \right) \leq \exp(-t).$$

Lemma B.2 (Bounds on ψ_2 -norm of Gaussians [33]). *1. If $X \sim \mathcal{N}(0, \sigma^2)$ is a centered Gaussian random variable with variance σ^2 , then its ψ_2 -norm (17) satisfies*

$$\|X\|_{\psi_2} \leq \sqrt{\frac{8}{3}}\sigma.$$

2. If $X \sim \mathcal{N}(\mu, \sigma^2)$ is a Gaussian random variable with mean μ and variance σ^2 , then its ψ_2 -norm (17) satisfies

$$\|X\|_{\psi_2} \leq \max \left(2\sigma, \sqrt{\frac{\mu^2}{\log 2} + \sigma^2} \right).$$

B.2 Proof of Theorem 3.1

Proof of Theorem 3.1. Given the output of an affine transformation $\mathbf{x} = \mathbf{W}\mathbf{v} + \mathbf{b}$, where \mathbf{W} and \mathbf{b} are learnable parameters. If $\mathbf{x}' = (\alpha\mathbf{W})\mathbf{v} + (\alpha\mathbf{b})$, then the output of UnitNorm is unchanged, i.e.,

$\tilde{\mathbf{x}}' = \tilde{\mathbf{x}}$, while the gradients to loss \mathcal{L} are given as follows:

$$\begin{aligned}\frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{x}}'} \cdot \frac{\partial \tilde{\mathbf{x}}'}{\partial (\alpha \mathbf{W})} &= \frac{1}{\alpha} \cdot \frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{x}}} \cdot \frac{\partial \tilde{\mathbf{x}}}{\partial \mathbf{W}} = \frac{1}{\alpha} \cdot \frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{x}}} \cdot \mathbf{J} \mathbf{v}^\top \\ \frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{x}}'} \cdot \frac{\partial \tilde{\mathbf{x}}'}{\partial (\alpha \mathbf{b})} &= \frac{1}{\alpha} \cdot \frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{x}}} \cdot \frac{\partial \tilde{\mathbf{x}}}{\partial \mathbf{b}} = \frac{1}{\alpha} \cdot \frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{x}}} \cdot \mathbf{J} \\ \frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{x}}'} \cdot \frac{\partial \tilde{\mathbf{x}}'}{\partial \mathbf{v}} &= \frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{x}}} \cdot \frac{\partial \tilde{\mathbf{x}}}{\partial \mathbf{v}} = \frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{x}}} \cdot \mathbf{J} \mathbf{W}^\top\end{aligned}\tag{20}$$

Proof: First we will show $\tilde{\mathbf{x}}' = \tilde{\mathbf{x}}$, for which we have:

$$\begin{aligned}\tilde{\mathbf{x}}' &= D^{\frac{k}{2}} \frac{\mathbf{x}'}{\|\mathbf{x}'\|} \\ &= D^{\frac{k}{2}} \frac{\alpha \mathbf{x}}{\alpha \|\mathbf{x}\|} \\ &= D^{\frac{k}{2}} \frac{\mathbf{x}}{\|\mathbf{x}\|} \\ &= \tilde{\mathbf{x}}\end{aligned}\tag{21}$$

And thus for the gradients to loss \mathcal{L} , we have $\frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{x}}'} = \frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{x}}}$. Also, for the Jacobian matrix \mathbf{J} of $\tilde{\mathbf{x}}$ w.r.t. \mathbf{x} , we have

$$\begin{aligned}\mathbf{J} &= \frac{\partial D^{\frac{k}{2}} \frac{\mathbf{x}}{\|\mathbf{x}\|}}{\partial \mathbf{x}} \\ &= D^{\frac{k}{2}} \left(\frac{\mathbf{I}}{\|\mathbf{x}\|} - \frac{\mathbf{x} \mathbf{x}^\top}{\|\mathbf{x}\|^3} \right)\end{aligned}\tag{22}$$

And the Jacobian matrix of $\tilde{\mathbf{x}}'$ w.r.t. \mathbf{x}' is given as:

$$\begin{aligned}\frac{\partial D^{\frac{k}{2}} \frac{\mathbf{x}'}{\|\mathbf{x}'\|}}{\partial \mathbf{x}'} &= D^{\frac{k}{2}} \left(\frac{\mathbf{I}}{\|\mathbf{x}'\|} - \frac{\mathbf{x}' \mathbf{x}'^\top}{\|\mathbf{x}'\|^3} \right) \\ &= D^{\frac{k}{2}} \left(\frac{\mathbf{I}}{\alpha \|\mathbf{x}\|} - \frac{\alpha^2 \mathbf{x} \mathbf{x}^\top}{\alpha^3 \|\mathbf{x}\|^3} \right) \\ &= \frac{1}{\alpha} D^{\frac{k}{2}} \left(\frac{\mathbf{I}}{\|\mathbf{x}\|} - \frac{\mathbf{x} \mathbf{x}^\top}{\|\mathbf{x}\|^3} \right) \\ &= \frac{1}{\alpha} \mathbf{J}\end{aligned}\tag{23}$$

Then we have the gradient of loss w.r.t. \mathbf{W} and $\alpha \mathbf{W}$:

$$\begin{aligned}\frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{x}}} \cdot \frac{\partial \tilde{\mathbf{x}}}{\partial \mathbf{W}} &= \frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{x}}} \cdot \frac{\partial \tilde{\mathbf{x}}}{\partial \mathbf{x}} \cdot \frac{\partial \mathbf{x}}{\partial \mathbf{W}} \\ &= \frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{x}}} \cdot \mathbf{J} \mathbf{v}^\top \\ \frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{x}}'} \cdot \frac{\partial \tilde{\mathbf{x}}'}{\partial (\alpha \mathbf{W})} &= \frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{x}}'} \cdot \frac{\partial \tilde{\mathbf{x}}'}{\partial \mathbf{x}'} \cdot \frac{\partial \mathbf{x}'}{\partial (\alpha \mathbf{W})} \\ &= \frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{x}}} \cdot \frac{1}{\alpha} \mathbf{J} \mathbf{v}^\top \\ \Rightarrow \frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{x}}'} \cdot \frac{\partial \tilde{\mathbf{x}}'}{\partial (\alpha \mathbf{W})} &= \frac{1}{\alpha} \cdot \frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{x}}} \cdot \frac{\partial \tilde{\mathbf{x}}}{\partial \mathbf{W}} = \frac{1}{\alpha} \cdot \frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{x}}} \cdot \mathbf{J} \mathbf{v}^\top\end{aligned}\tag{24}$$

Similarly, for \mathbf{b} and $\alpha\mathbf{b}$ we have:

$$\begin{aligned}
\frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{x}}} \cdot \frac{\partial \tilde{\mathbf{x}}}{\partial \mathbf{b}} &= \frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{x}}} \cdot \frac{\partial \tilde{\mathbf{x}}}{\partial \mathbf{x}} \cdot \frac{\partial \mathbf{x}}{\partial \mathbf{b}} \\
&= \frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{x}}} \cdot \mathbf{J} \\
\frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{x}}'} \cdot \frac{\partial \tilde{\mathbf{x}}'}{\partial (\alpha\mathbf{b})} &= \frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{x}}'} \cdot \frac{\partial \tilde{\mathbf{x}}'}{\partial \mathbf{x}'} \cdot \frac{\partial \mathbf{x}'}{\partial (\alpha\mathbf{b})} \\
&= \frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{x}}} \cdot \frac{1}{\alpha} \mathbf{J} \\
\Rightarrow \frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{x}}'} \cdot \frac{\partial \tilde{\mathbf{x}}'}{\partial (\alpha\mathbf{b})} &= \frac{1}{\alpha} \cdot \frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{x}}} \cdot \frac{\partial \tilde{\mathbf{x}}}{\partial \mathbf{b}} = \frac{1}{\alpha} \cdot \frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{x}}} \cdot \mathbf{J}
\end{aligned} \tag{25}$$

And for \mathbf{v} , we have:

$$\begin{aligned}
\frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{x}}} \cdot \frac{\partial \tilde{\mathbf{x}}}{\partial \mathbf{v}} &= \frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{x}}} \cdot \frac{\partial \tilde{\mathbf{x}}}{\partial \mathbf{x}} \cdot \frac{\partial \mathbf{x}}{\partial \mathbf{v}} \\
&= \frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{x}}} \cdot \mathbf{J} \mathbf{W}^\top \\
\frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{x}}'} \cdot \frac{\partial \tilde{\mathbf{x}}'}{\partial \mathbf{v}} &= \frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{x}}'} \cdot \frac{\partial \tilde{\mathbf{x}}'}{\partial \mathbf{x}'} \cdot \frac{\partial \mathbf{x}'}{\partial \mathbf{v}} \\
&= \frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{x}}} \cdot \frac{1}{\alpha} \mathbf{J} (\alpha \mathbf{W})^\top \\
\Rightarrow \frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{x}}'} \cdot \frac{\partial \tilde{\mathbf{x}}'}{\partial \mathbf{v}} &= \frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{x}}} \cdot \frac{\partial \tilde{\mathbf{x}}}{\partial \mathbf{v}} = \frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{x}}} \cdot \mathbf{J} \mathbf{W}^\top
\end{aligned} \tag{26}$$

□

B.3 Proofs of Theorem 3.2 and Corollary 3.3

Proof of Theorem 3.2. Let $\mathbf{X} \in \mathbb{R}^{L \times D}$ be a single sequence of token vectors, and let $\tilde{\mathbf{X}}$ be the unit normalized output with modulus k , the entropy lower bound (ELB) of the attention scores is given by the following expression:

$$\begin{aligned}
\text{ELB}(k; L, D) &= \min_{i=1}^L H(\mathbf{A}_i) \\
&= \min_{i=1}^L \left(- \sum_{j=1}^L \mathbf{A}_{i,j} \log \mathbf{A}_{i,j} \right) \\
&= \log \left(L - 1 + \exp \left(2D^{k-\frac{1}{2}} \right) \right) - \frac{2D^{k-\frac{1}{2}} \exp \left(2D^{k-\frac{1}{2}} \right)}{L - 1 + \exp \left(2D^{k-\frac{1}{2}} \right)}
\end{aligned} \tag{27}$$

Proof: Let $\tilde{\mathbf{X}} = D^{\frac{k}{2}} \mathbf{e}$ where \mathbf{e} are the vectors of unit norm. Without loss of generality, we can assume the ELB is achieved at anchor index i , where we can compute the attention scores as follows:

$$\begin{aligned}
\mathbf{A}_i &= \text{softmax} \left(\frac{\tilde{\mathbf{X}}_i \tilde{\mathbf{X}}^\top}{\sqrt{D}} \right) \\
&= \text{softmax} \left(\frac{D^k \mathbf{e}_i \mathbf{e}^\top}{\sqrt{D}} \right) \\
&= \text{softmax} \left(D^{k-\frac{1}{2}} \mathbf{e}_i \mathbf{e}^\top \right)
\end{aligned} \tag{28}$$

Since $\mathbf{e}_i \mathbf{e}_j^\top \in (-1, 1)$, $\forall i, j = 1, 2, \dots, L$, the entropy of the attentions scores is lower bounded by the following expression when it satisfies that $\mathbf{e}_i \mathbf{e}_j = \begin{cases} 1, & j = i \\ -1, & j \neq i \end{cases}$:

$$\begin{aligned}
& H(\mathbf{A}_i) \\
&= - \sum_{j=1}^L \mathbf{A}_{i,j} \log \mathbf{A}_{i,j} \\
&= -(L-1) \cdot \frac{\exp\left(-D^{k-\frac{1}{2}}\right)}{(L-1) \exp\left(-D^{k-\frac{1}{2}}\right) + \exp\left(D^{k-\frac{1}{2}}\right)} \log \frac{\exp\left(-D^{k-\frac{1}{2}}\right)}{(L-1) \exp\left(-D^{k-\frac{1}{2}}\right) + \exp\left(D^{k-\frac{1}{2}}\right)} \\
&\quad - \frac{\exp\left(D^{k-\frac{1}{2}}\right)}{(L-1) \exp\left(-D^{k-\frac{1}{2}}\right) + \exp\left(D^{k-\frac{1}{2}}\right)} \log \frac{\exp\left(D^{k-\frac{1}{2}}\right)}{(L-1) \exp\left(-D^{k-\frac{1}{2}}\right) + \exp\left(D^{k-\frac{1}{2}}\right)} \\
&= \frac{L-1}{L-1 + \exp\left(2D^{k-\frac{1}{2}}\right)} \log\left(L-1 + \exp\left(2D^{k-\frac{1}{2}}\right)\right) \\
&\quad + \frac{\exp\left(2D^{k-\frac{1}{2}}\right)}{L-1 + \exp\left(2D^{k-\frac{1}{2}}\right)} \log \frac{L-1 + \exp\left(2D^{k-\frac{1}{2}}\right)}{\exp\left(2D^{k-\frac{1}{2}}\right)} \\
&= \log\left(L-1 + \exp\left(2D^{k-\frac{1}{2}}\right)\right) - \frac{2D^{k-\frac{1}{2}} \exp\left(2D^{k-\frac{1}{2}}\right)}{L-1 + \exp\left(2D^{k-\frac{1}{2}}\right)}
\end{aligned} \tag{29}$$

Therefore, the entropy lower bound (ELB) for any L, D and k is:

$$\text{ELB}(k; L, D) = \log\left(L-1 + \exp\left(2D^{k-\frac{1}{2}}\right)\right) - \frac{2D^{k-\frac{1}{2}} \exp\left(2D^{k-\frac{1}{2}}\right)}{L-1 + \exp\left(2D^{k-\frac{1}{2}}\right)} \tag{30}$$

□

Proof of Corollary 3.3. The ELB is a monotonically decreasing function of k bounded between 0 and $\log L$.

Proof: Let $d = 2D^{k-\frac{1}{2}}$, then it is obvious that d is monotonically increasing with k , therefore we only need to prove that $\text{ELB}(k; L, D)$ is monotonically decreasing with d . The derivative of $\text{ELB}(k; L, D)$ with respect to d is given as follows:

$$\begin{aligned}
\frac{\partial \text{ELB}(k; L, D)}{\partial d} &= \frac{e^d}{L-1 + e^d} - \frac{(L-1 + e^d)(d+1)e^d - (de^d)e^d}{(L-1 + e^d)^2} \\
&= \frac{e^d}{(L-1 + e^d)^2} ((L-1 + e^d) - (L-1 + e^d)(d+1) + de^d) \\
&= \frac{de^d}{(L-1 + e^d)^2} (1-L) \\
&(\forall L > 1) < 0
\end{aligned} \tag{31}$$

Therefore, $\text{ELB}(k; L, D)$ is monotonically decreasing with d and with k . If the limits of $\text{ELB}(k; L, D)$ as $k \rightarrow -\infty$ and $k \rightarrow +\infty$ exist, then $\text{ELB}(k; L, D)$ is bounded between these two limits. The limits are given as follows:

$$\begin{aligned}
\lim_{k \rightarrow -\infty} \text{ELB}(k; L, D) &= \lim_{d \rightarrow 0^+} \left(\log(L-1 + e^d) - \frac{de^d}{L-1 + e^d} \right) \\
&= \log(L-1 + 1) - \frac{0}{L-1 + 1} \\
&= \log L
\end{aligned} \tag{32}$$

$$\begin{aligned}
\lim_{k \rightarrow +\infty} \text{ELB}(k; L, D) &= \lim_{d \rightarrow +\infty} \left(\log(L - 1 + e^d) - \frac{de^d}{L - 1 + e^d} \right) \\
&= \lim_{d \rightarrow +\infty} \log e^d - \lim_{d \rightarrow +\infty} \frac{d}{(L - 1)e^{-d} + 1} \\
&= d - d \\
&= 0
\end{aligned} \tag{33}$$

Therefore, $\text{ELB}(k; L, D)$ is bounded between 0 and $\log L$. \square

C Discussion

C.1 Difference between the proposed normalization and the other normalization

BatchNorm and LayerNorm are all normalization methods that are widely used in deep learning. They share the same center-and-scale normalization paradigm by first subtracting the mean and then divide by standard deviation. The only difference between them in terms of computation is the dimensions of data used to compute these statistics, as shown in Table S1.

In terms of application, BatchNorm is often used in fully connected layers and convolution layers, while LayerNorm is often used in recurrent neural networks and Transformers. The subtle difference between LayerNorm (theory) and LayerNorm (practice) might be attributed to the fact that the sequence length L is often variable in Transformers, thus normalization within each token might be more stable. But this will require further investigation to come to a conclusion.

The proposed UnitNorm is a normalization method that is used to normalize the input data to have unit norm, which takes the same dimension for computation as LayerNorm, yet it distinguishes itself from LayerNorm by the fact that it does not subtract the mean and divide by standard deviation. Also, UnitNorm discard the center operation on the normalized output, as it will also cause the problem of token shift (Section 2.1).

C.2 Feasibility of switching the order of normalization and projection in theoretical analysis

Let $\mathbf{X} \in \mathbb{R}^{L \times D}$ be a single sequence of token vectors, and the normalization operation is given in the following form:

$$f : \mathbf{X} \mapsto \frac{\mathbf{X} - \boldsymbol{\mu}}{\boldsymbol{\sigma}} \equiv \mathbf{X}\mathbf{W} + \mathbf{b} \tag{34}$$

where $\boldsymbol{\mu}$ and $\boldsymbol{\sigma}$ are the mean and standard deviation of the input vector \mathbf{X} , respectively, and $\mathbf{W} = \boldsymbol{\sigma}^{-1}$ and $\mathbf{b} = \boldsymbol{\mu}\boldsymbol{\sigma}^{-1}$. Depending on the normalization method, the mean and standard deviation can be computed over different dimensions.

The projection in the attention mechanism maps the input vectors to query, key and value vectors, and here we only consider the query and key vectors for this discussion, which are computed as follows:

$$\begin{aligned}
\mathbf{Q} &= \mathbf{X}\mathbf{W}_Q + \mathbf{b}_Q \\
\mathbf{K} &= \mathbf{X}\mathbf{W}_K + \mathbf{b}_K
\end{aligned} \tag{35}$$

where $\mathbf{W}_Q, \mathbf{W}_K \in \mathbb{R}^{D \times D}$ are the projection matrices and $\mathbf{b}_Q, \mathbf{b}_K \in \mathbb{R}^D$ are the bias vectors for query and key, respectively. As the normalization and projection are both linear operations, we can combine them into a single linear operation as follows:

$$\begin{aligned}
\mathbf{Y} &= \tilde{\mathbf{X}}\mathbf{W}_Y + \mathbf{b}_Y \\
&= (\mathbf{X}\mathbf{W} + \mathbf{b})\mathbf{W}_Y + \mathbf{b}_Y \\
&= \mathbf{X}(\mathbf{W}\mathbf{W}_Y) + (\mathbf{b}\mathbf{W}_Y + \mathbf{b}_Y)
\end{aligned} \tag{36}$$

for $Y \in \{Q, K\}$. Therefore, there must exist some \mathbf{W}' , \mathbf{b}' , \mathbf{W}'_Y and \mathbf{b}'_Y such that:

$$\begin{aligned}
\mathbf{W}'_Y\mathbf{W}' &= \mathbf{W}\mathbf{W}_Y \\
\mathbf{b}_Y\mathbf{W}' + \mathbf{b}' &= \mathbf{b}\mathbf{W}_Y + \mathbf{b}_Y
\end{aligned} \tag{37}$$

Table S1: Computation of the statistics for different normalization methods. Input data $\mathbf{X} \in \mathbb{R}^{N \times L \times D}$, where N is the batch size, L is the sequence length and D is the feature dimension. $\mathbf{X}_{n,l,d}$ denotes the d -th feature of the l -th token in the n -th sequence. Normalization is broadcasted over the same dimension as the statistics and mathematical operations are done element-wise. For BatchNorm, LayerNorm (theory) and LayerNorm (practice), γ and β are optional learnable parameters that will re-scale and re-center the normalized output element-wise, which is enabled by default in the PyTorch’s implementation.

| Method | Statistics | Normalization |
|----------------------|--|--|
| BatchNorm | $\mu_d = \frac{1}{NL} \sum_{n=1}^N \sum_{l=1}^L \mathbf{X}_{n,l,d}$ $\sigma_d^2 = \frac{1}{NL} \sum_{n=1}^N \sum_{l=1}^L (\mathbf{X}_{n,l,d} - \mu_d)^2$ $\boldsymbol{\mu} = [\mu_1 \quad \mu_2 \quad \cdots \quad \mu_D]^\top \in \mathbb{R}^{1 \times 1 \times D}$ $\boldsymbol{\sigma}^2 = [\sigma_1^2 \quad \sigma_2^2 \quad \cdots \quad \sigma_D^2]^\top \in \mathbb{R}^{1 \times 1 \times D}$ | |
| LayerNorm (theory) | $\mu_n = \frac{1}{LD} \sum_{l=1}^L \sum_{d=1}^D \mathbf{X}_{n,l,d}$ $\sigma_n^2 = \frac{1}{LD} \sum_{l=1}^L \sum_{d=1}^D (\mathbf{X}_{n,l,d} - \mu_n)^2$ $\boldsymbol{\mu} = [\mu_1 \quad \mu_2 \quad \cdots \quad \mu_N]^\top \in \mathbb{R}^{N \times 1 \times 1}$ $\boldsymbol{\sigma}^2 = [\sigma_1^2 \quad \sigma_2^2 \quad \cdots \quad \sigma_N^2]^\top \in \mathbb{R}^{N \times 1 \times 1}$ | $\tilde{\mathbf{X}} = \frac{\mathbf{X} - \boldsymbol{\mu}}{\sqrt{\boldsymbol{\sigma}^2 + \varepsilon}}$ $\mathbf{Y} = \tilde{\mathbf{X}} \odot \boldsymbol{\gamma} + \boldsymbol{\beta}$ |
| LayerNorm (practice) | $\mu_{n,l} = \frac{1}{D} \sum_{d=1}^D \mathbf{X}_{n,l,d}$ $\sigma_{n,l}^2 = \frac{1}{D} \sum_{d=1}^D (\mathbf{X}_{n,l,d} - \mu_{n,l})^2$ $\boldsymbol{\mu} = \begin{bmatrix} \mu_{1,1} & \mu_{1,2} & \cdots & \mu_{1,L} \\ \mu_{2,1} & \mu_{2,2} & \cdots & \mu_{2,L} \\ \vdots & \vdots & \ddots & \vdots \\ \mu_{N,1} & \mu_{N,2} & \cdots & \mu_{N,L} \end{bmatrix}^\top \in \mathbb{R}^{N \times L \times 1}$ $\boldsymbol{\sigma}^2 = \begin{bmatrix} \sigma_{1,1}^2 & \sigma_{1,2}^2 & \cdots & \sigma_{1,L}^2 \\ \sigma_{2,1}^2 & \sigma_{2,2}^2 & \cdots & \sigma_{2,L}^2 \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{N,1}^2 & \sigma_{N,2}^2 & \cdots & \sigma_{N,L}^2 \end{bmatrix}^\top \in \mathbb{R}^{N \times L \times 1}$ | |
| RMSNorm | $\ \mathbf{X}\ _{n,l} = \sqrt{\sum_{d=1}^D \mathbf{X}_{n,l,d}^2}$ | $\tilde{\mathbf{X}} = \sqrt{D} \frac{\mathbf{X}}{\ \mathbf{X}\ }$ $\mathbf{Y} = \tilde{\mathbf{X}} \odot \boldsymbol{\gamma} + \boldsymbol{\beta}$ |
| UnitNorm | $\ \mathbf{X}\ = \begin{bmatrix} \ \mathbf{X}\ _{1,1} & \ \mathbf{X}\ _{1,2} & \cdots & \ \mathbf{X}\ _{1,L} \\ \ \mathbf{X}\ _{2,1} & \ \mathbf{X}\ _{2,2} & \cdots & \ \mathbf{X}\ _{2,L} \\ \vdots & \vdots & \ddots & \vdots \\ \ \mathbf{X}\ _{N,1} & \ \mathbf{X}\ _{N,2} & \cdots & \ \mathbf{X}\ _{N,L} \end{bmatrix}^\top$ $\in \mathbb{R}^{N \times L \times 1}$ | $\tilde{\mathbf{X}} = D^{\frac{1}{2}} \frac{\mathbf{X}}{\ \mathbf{X}\ }$ $\mathbf{Y} = \tilde{\mathbf{X}}$ |

Therefore, the order of normalization and projection does not affect the theoretical analysis. And in favor of simplicity, we can assume the normalization is performed after the projection.

D Supplementary Figures

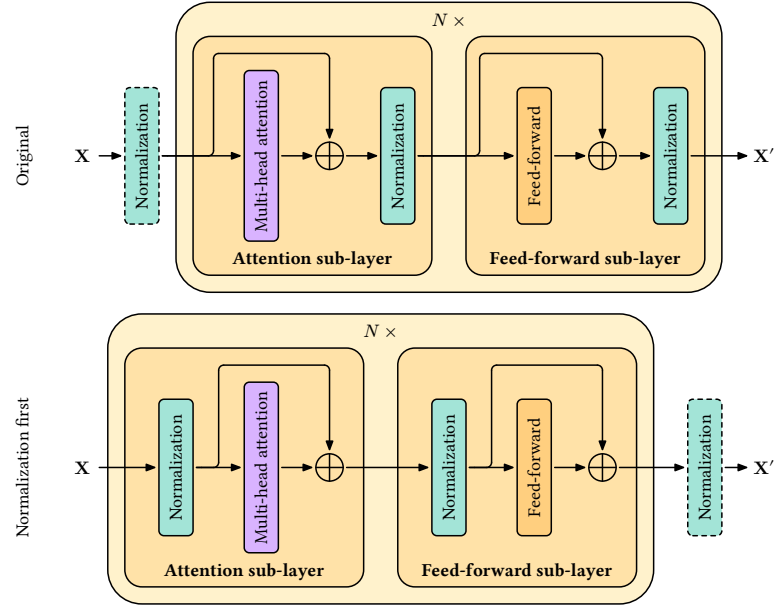


Figure S1: Transformer layer architecture. The original architecture is equivalent to a normalization-first sub-layer design for simpler analysis.

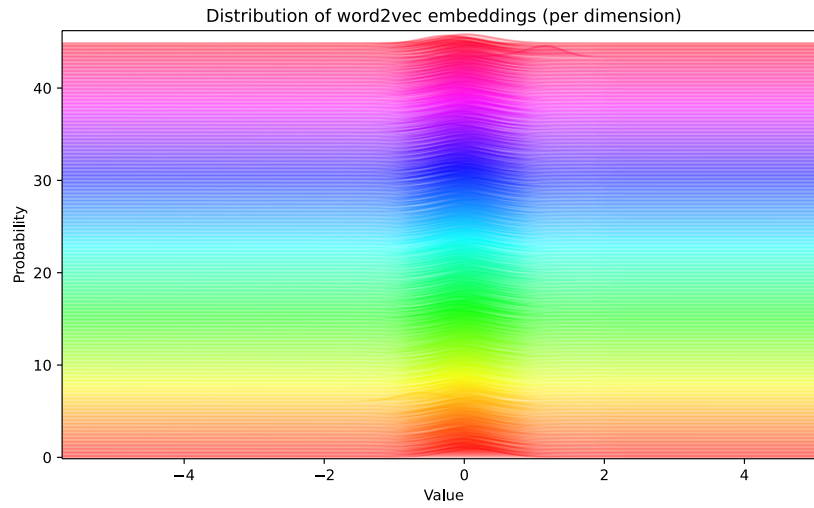


Figure S2: Distribution of values in each dimension of the word2vec embedding. The word2vec embedding is a 300-dimensional vector, and the distribution follows a normal distribution with means mostly around 0.

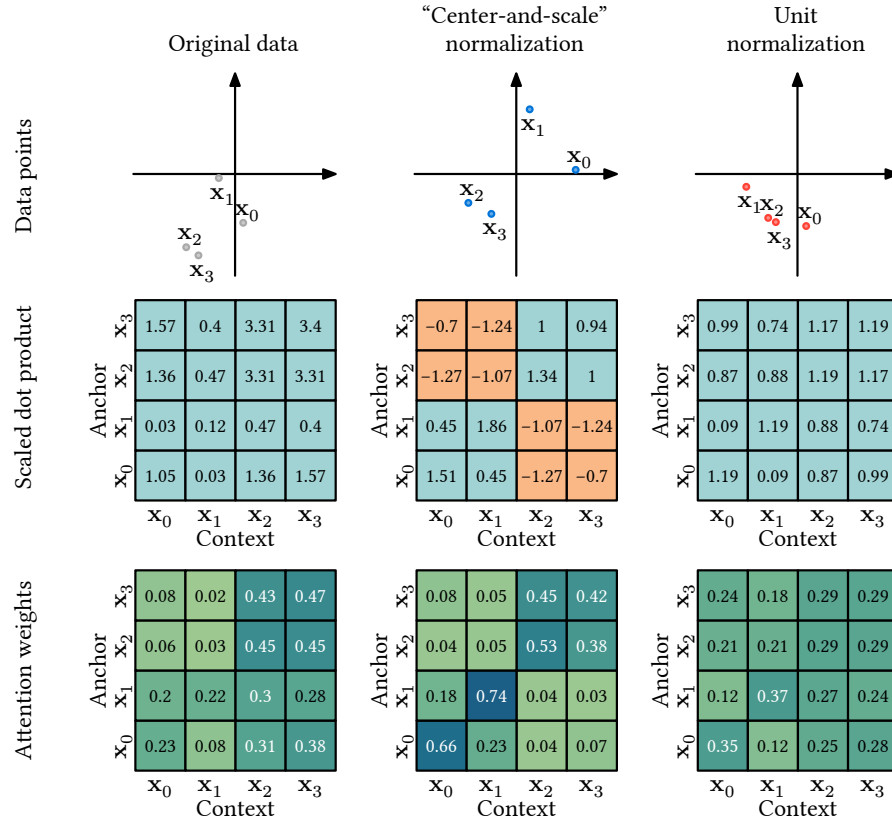


Figure S3: Demonstration of the token shift and attention shift problems using artificial data. The x_0 and x_1 exhibit typical token shift as shifting away from their original quadrants, resulting in sign flip in scaled dot product (marked in orange), and leading to less attention weights distributed to x_2 and x_3 than original. Attention shift and sparse attention problem can also be observed as the maximum attention weight is altered from x_2 and x_3 to nearly solely onto themselves.

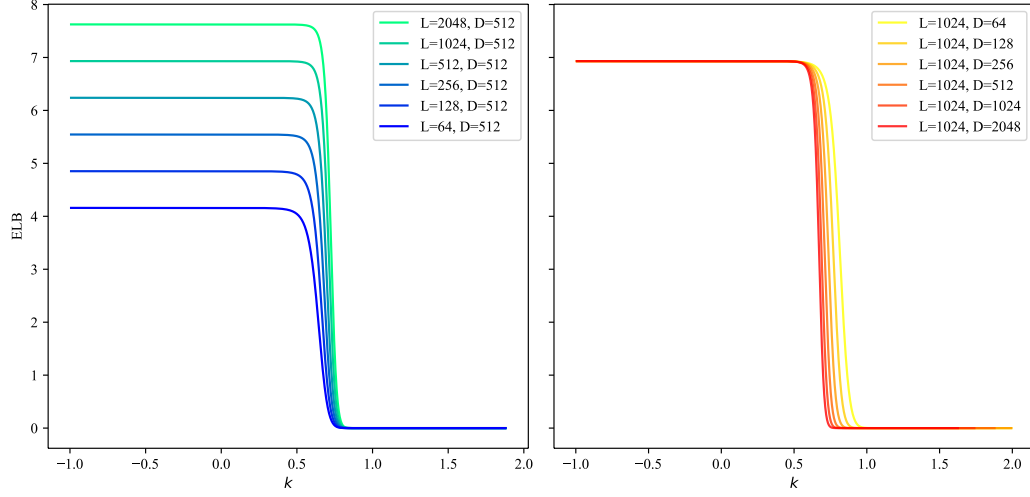


Figure S4: Entropy lower bound (ELB) against k for different L, D . The left figure shows the curve for fixed $D = 512$ and varying L , and the right figure shows the curve for fixed $L = 1024$ and varying D .

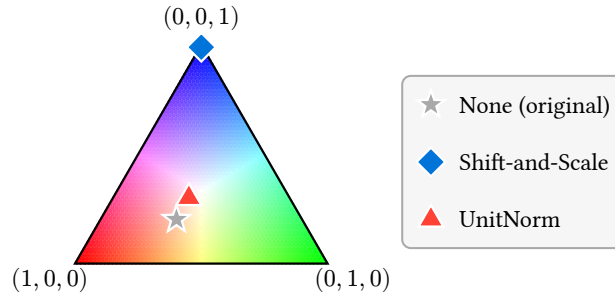


Figure S5: Graphical representation of attention weights showing a simple scenario of 3 tokens. Each corner represents a one-hot distribution (red, blue and green) and the center representing a uniform distribution (white). Gray star, blue diamond, and red triangle mark the attention weights with no normalization, center-and-scale normalization, and UnitNorm, respectively.

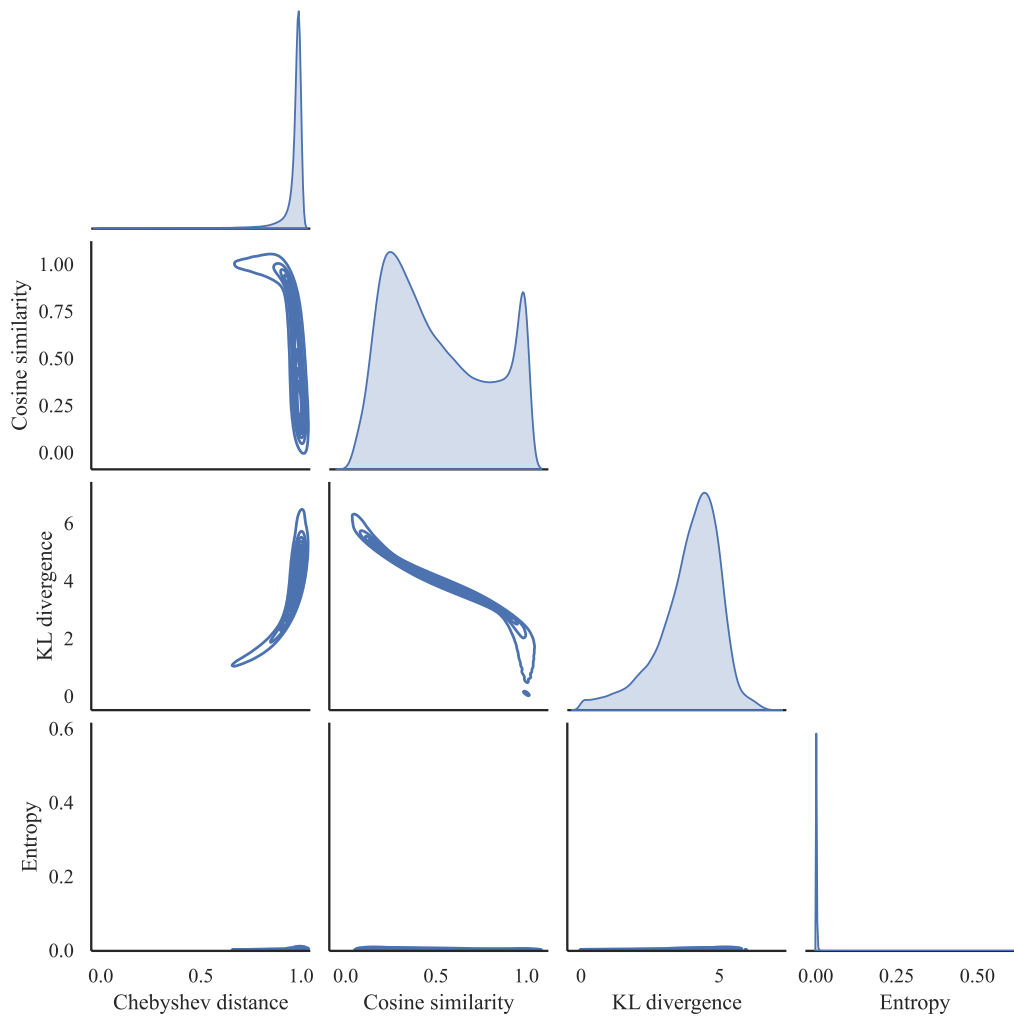


Figure S6: Joint distribution of metrics for LayerNorm (practice). Metrics used are defined as in Table S9.

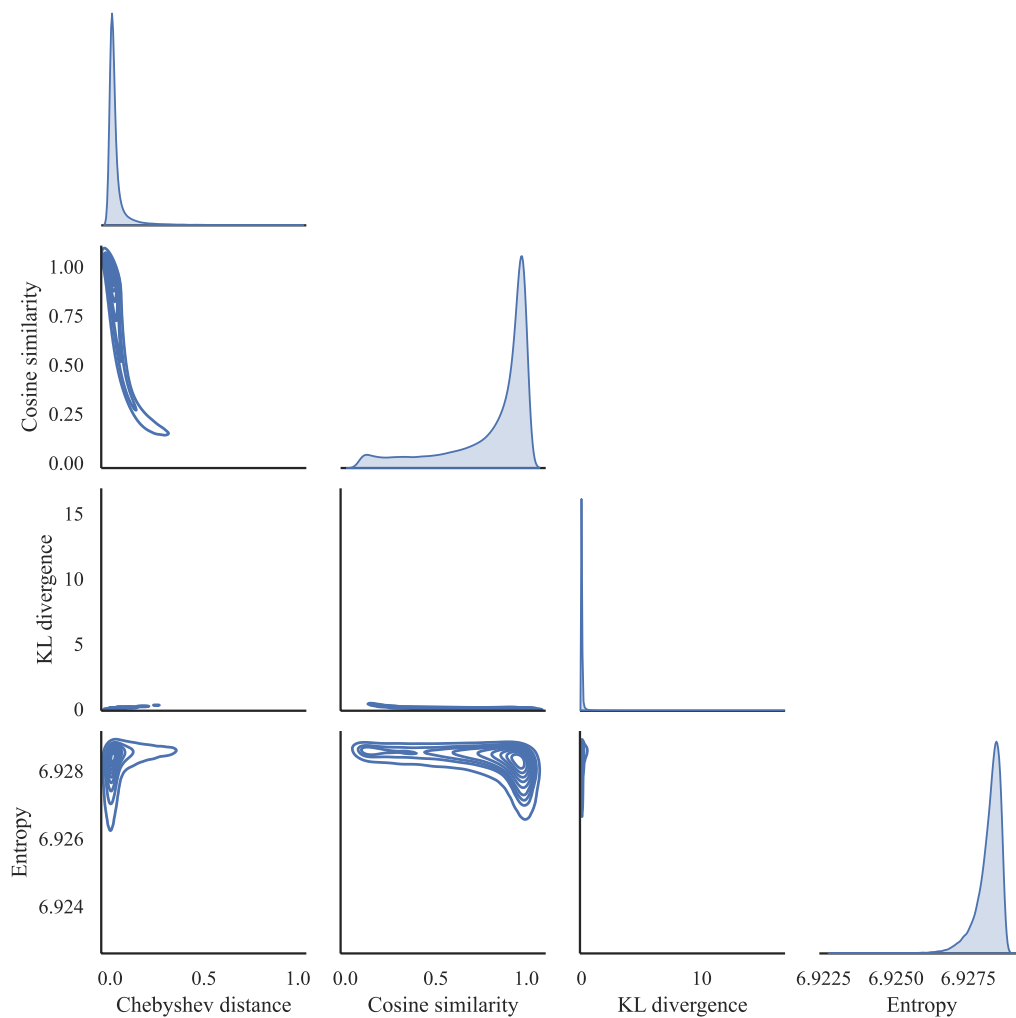


Figure S7: Joint distribution of metrics for UnitNorm. Metrics used are defined as in Table S9.

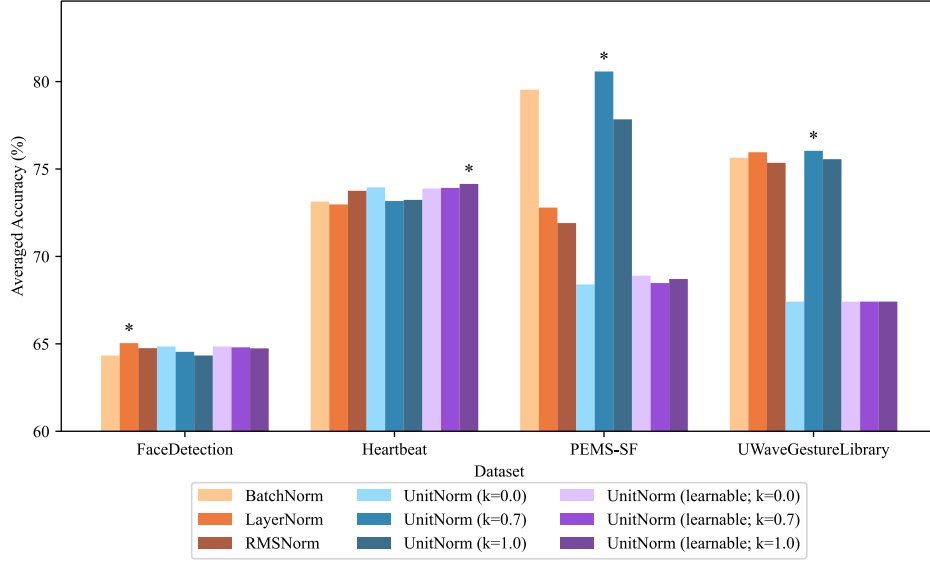


Figure S8: Average rank of normalization methods on the classification tasks. X-axis: Dataset with different normalization, Y-axis: average rank over models. Ranks are computed based on the accuracy of each model on each task with different normalization methods (lower is better). * indicates the best performing normalization method(s) on each task. UnitNorm and UnitNorm (learnable) outperform other normalization methods on 3 out of 5 datasets, showing its potential in classification tasks.

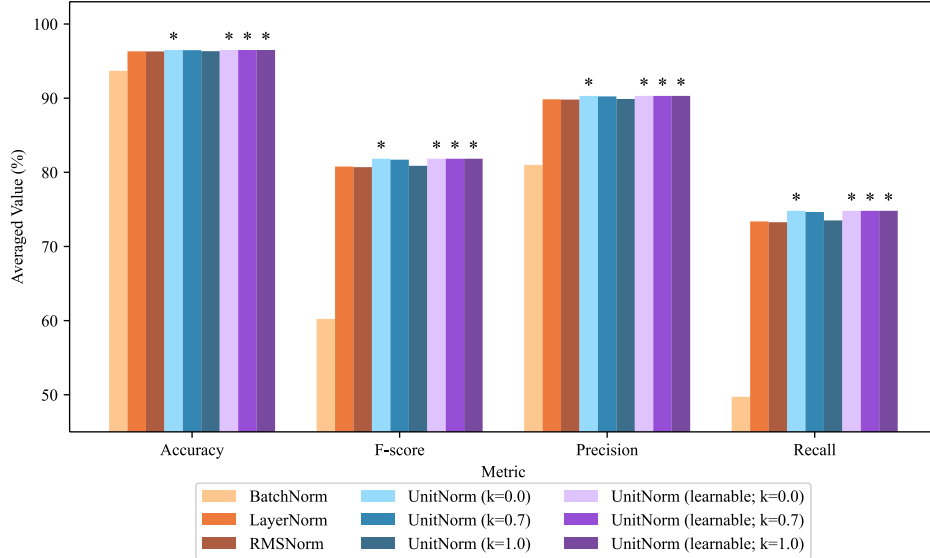


Figure S9: Average rank of normalization methods on the anomaly detection tasks. X-axis: Metrics under different normalization, Y-axis: average rank over models. Ranks are computed based on every metric of each model with different normalization methods (lower is better). * indicates the best performing normalization method(s) on each metric. UnitNorm and UnitNorm (learnable) show a dominating performance gain over the other normalization methods in all metrics.

E Supplementary Tables

Table S2: Summary of long term forecasting benchmark settings. The sequence length is the number of historical time steps fed into the encoder, and the label length is the number of time steps fed into the decoder as the ground truth output of the decoder. The prediction length is the number of time steps to be predicted by the decoder.

| Datasets | Feature number | Sequence length | Label length | Prediction length | Metrics | License |
|-------------------|----------------|-----------------|--------------|-------------------|----------|--------------|
| ETTh1, ETTh2 [22] | 7 | 384 | 96 | 96, 192, 384, 720 | MSE, MAE | CC BY-ND 4.0 |
| ECL [35] | 321 | | | | | CC BY 4.0 |
| Exchange [36] | 8 | | | | | N/A |

Table S3: Summary of classification benchmark settings. All datasets are from UEA Archive [37]. The sequence length is the number of time steps in each sequence fed into the encoder, and the prediction is made on the flattened output of the encoder by a fully connected layer.

| Datasets | Feature number | Class number | Sequence length | Metrics | License |
|---------------------|----------------|--------------|-----------------|----------|---------|
| FaceDetection | 144 | 5890 | 96 | Accuracy | N/A |
| Heartbeat | 61 | 204 | | | |
| PEMS-SF | 963 | 173 | | | |
| UWaveGestureLibrary | 3 | 320 | | | |

Table S4: Summary of anomaly detection benchmark settings. The sequence length is the number of time steps in each sequence fed into the model for reconstruction using MSE as loss. The threshold is determined by the distribution of reconstruction error on the training set, and the metrics are computed on the test set based on this threshold.

| Datasets | Feature number | Sequence length | Reconstruction error | Metrics | License |
|----------|----------------|-----------------|----------------------|---------------------------------------|---------|
| MSL [38] | 55 | 100 | MSE | Accuracy, F1-score, Precision, Recall | N/A |

Table S5: Summary of compute resources used for the experiments. Depending on the dataset and model, the GPU memory usage varies from 4G to 64G.

| CPU | Memory | GPU | GPU Memory |
|-------------------------|--------|----------------------|------------|
| AMD Threadripper 3995WX | 512G | 4 × NVIDIA RTX A5000 | 4 × 24G |

Table S6: Long term forecasting test losses on different datasets using different models and normalization methods. For each dataset, prediction length, metric and for each model, the best performing normalization method(s) are bolded, and the second best are underlined.

| dataset | ECL | | | | ETTh1 | | | | ETTh2 | | | | Exchange | | | |
|------------------|-------------------|--------------|--------------|--------------|-------------------|--------------|--|--|-------------------|--------------|--------------|--------------|-------------------|--|--|--|
| | prediction length | | | | prediction length | | | | prediction length | | | | prediction length | | | |
| | metric | | | | metric | | | | metric | | | | metric | | | |
| BatchNorm | Crossformer | 0.408 | 0.278 | 0.435 | 0.311 | 0.246 | | | 0.408 | 0.278 | 0.435 | 0.311 | 0.246 | | | |
| | FEDformer | 0.310 | 0.184 | 0.357 | 0.198 | 0.144 | | | 0.310 | 0.184 | 0.357 | 0.198 | 0.144 | | | |
| | Informer | 0.409 | 0.285 | 0.448 | 0.322 | 0.265 | | | 0.409 | 0.285 | 0.448 | 0.322 | 0.265 | | | |
| | PatchTST | 0.321 | 0.191 | 0.364 | 0.211 | 0.162 | | | 0.321 | 0.191 | 0.364 | 0.211 | 0.162 | | | |
| | Transformer | 0.463 | 0.300 | 0.455 | 0.342 | 0.290 | | | 0.463 | 0.300 | 0.455 | 0.342 | 0.290 | | | |
| | | 0.407 | 0.207 | 0.376 | 0.234 | 0.189 | | | 0.407 | 0.207 | 0.376 | 0.234 | 0.189 | | | |
| LayerNorm | Crossformer | 0.510 | 0.332 | 0.478 | 0.372 | 0.338 | | | 0.510 | 0.332 | 0.478 | 0.372 | 0.338 | | | |
| | FEDformer | 0.461 | 0.248 | 0.417 | 0.270 | 0.255 | | | 0.461 | 0.248 | 0.417 | 0.270 | 0.255 | | | |
| | Informer | 0.814 | 0.395 | 0.661 | 0.422 | 0.426 | | | 0.814 | 0.395 | 0.661 | 0.422 | 0.426 | | | |
| | PatchTST | 1.008 | 0.374 | 0.790 | 0.389 | 0.417 | | | 1.008 | 0.374 | 0.790 | 0.389 | 0.417 | | | |
| | Transformer | 0.805 | 0.429 | 0.792 | 0.449 | 0.507 | | | 0.805 | 0.429 | 0.792 | 0.449 | 0.507 | | | |
| | | 1.014 | 0.426 | 1.015 | 0.433 | 0.531 | | | 1.014 | 0.426 | 1.015 | 0.433 | 0.531 | | | |
| RMSNorm | Crossformer | 0.886 | 0.462 | 0.886 | 0.477 | 0.620 | | | 0.886 | 0.462 | 0.886 | 0.477 | 0.620 | | | |
| | FEDformer | 1.161 | 0.478 | 1.230 | 0.483 | 0.684 | | | 1.161 | 0.478 | 1.230 | 0.483 | 0.684 | | | |
| | Informer | 0.819 | 0.497 | 0.940 | 0.507 | 0.707 | | | 0.819 | 0.497 | 0.940 | 0.507 | 0.707 | | | |
| | PatchTST | 1.054 | 0.506 | 1.357 | 0.516 | 0.834 | | | 1.054 | 0.506 | 1.357 | 0.516 | 0.834 | | | |
| | Transformer | 1.093 | 0.346 | 1.414 | 0.395 | 0.557 | | | 1.093 | 0.346 | 1.414 | 0.395 | 0.557 | | | |
| | | 1.852 | 0.292 | 3.319 | 0.352 | 0.563 | | | 1.852 | 0.292 | 3.319 | 0.352 | 0.563 | | | |
| UnitNorm (k=0.0) | Crossformer | 1.258 | 0.399 | 2.105 | 0.434 | 0.878 | | | 1.258 | 0.399 | 2.105 | 0.434 | 0.878 | | | |
| | FEDformer | 2.488 | 0.376 | 6.878 | 0.423 | 1.355 | | | 2.488 | 0.376 | 6.878 | 0.423 | 1.355 | | | |
| | Informer | 1.603 | 0.435 | 2.215 | 0.473 | 0.961 | | | 1.603 | 0.435 | 2.215 | 0.473 | 0.961 | | | |
| | PatchTST | 3.874 | 0.421 | 6.966 | 0.469 | 1.626 | | | 3.874 | 0.421 | 6.966 | 0.469 | 1.626 | | | |
| | Transformer | 1.833 | 0.453 | 2.307 | 0.486 | 1.491 | | | 1.833 | 0.453 | 2.307 | 0.486 | 1.491 | | | |
| | | 4.782 | 0.435 | 8.194 | 0.479 | 3.213 | | | 4.782 | 0.435 | 8.194 | 0.479 | 3.213 | | | |
| Crossformer | Crossformer | 0.608 | 0.204 | 0.672 | 0.297 | 0.265 | | | 0.608 | 0.204 | 0.672 | 0.297 | 0.265 | | | |
| | FEDformer | 0.665 | 0.088 | 0.770 | 0.169 | 0.122 | | | 0.665 | 0.088 | 0.770 | 0.169 | 0.122 | | | |
| | Informer | 0.921 | 0.300 | 0.861 | 0.383 | 0.445 | | | 0.921 | 0.300 | 0.861 | 0.383 | 0.445 | | | |
| | PatchTST | 1.458 | 0.180 | 1.308 | 0.276 | 0.315 | | | 1.458 | 0.180 | 1.308 | 0.276 | 0.315 | | | |
| | Transformer | 1.242 | 0.419 | 1.367 | 0.487 | 0.646 | | | 1.242 | 0.419 | 1.367 | 0.487 | 0.646 | | | |
| | | 2.578 | 0.336 | 3.221 | 0.438 | 0.658 | | | 2.578 | 0.336 | 3.221 | 0.438 | 0.658 | | | |
| FEDformer | Crossformer | 1.444 | 0.703 | 1.602 | 0.823 | 0.846 | | | 1.444 | 0.703 | 1.602 | 0.823 | 0.846 | | | |
| | FEDformer | 3.069 | 0.874 | 4.284 | 1.151 | 1.086 | | | 3.069 | 0.874 | 4.284 | 1.151 | 1.086 | | | |
| | Informer | 0.589 | 0.209 | 0.733 | 0.297 | 0.378 | | | 0.589 | 0.209 | 0.733 | 0.297 | 0.378 | | | |
| | PatchTST | 0.581 | 0.091 | 0.830 | 0.169 | 0.274 | | | 0.581 | 0.091 | 0.830 | 0.169 | 0.274 | | | |
| | Transformer | 0.786 | 0.301 | 0.836 | 0.383 | 0.531 | | | 0.786 | 0.301 | 0.836 | 0.383 | 0.531 | | | |
| | | 1.047 | 0.180 | 1.081 | 0.276 | 0.502 | | | 1.047 | 0.180 | 1.081 | 0.276 | 0.502 | | | |
| Informer | Crossformer | 1.051 | 0.411 | 1.077 | 0.488 | 0.890 | | | 1.051 | 0.411 | 1.077 | 0.488 | 0.890 | | | |
| | FEDformer | 1.745 | 0.324 | 1.817 | 0.440 | 1.288 | | | 1.745 | 0.324 | 1.817 | 0.440 | 1.288 | | | |
| | Informer | 1.212 | 0.713 | 1.409 | 0.824 | 1.047 | | | 1.212 | 0.713 | 1.409 | 0.824 | 1.047 | | | |
| | PatchTST | 2.297 | 0.901 | 2.967 | 1.153 | 1.701 | | | 2.297 | 0.901 | 2.967 | 1.153 | 1.701 | | | |
| | Transformer | 1.188 | 0.345 | 1.502 | 0.395 | 0.721 | | | 1.188 | 0.345 | 1.502 | 0.395 | 0.721 | | | |
| | | 2.205 | 0.297 | 3.574 | 0.351 | 1.014 | | | 2.205 | 0.297 | 3.574 | 0.351 | 1.014 | | | |
| PatchTST | Crossformer | 1.820 | 0.399 | 2.056 | 0.438 | 0.909 | | | 1.820 | 0.399 | 2.056 | 0.438 | 0.909 | | | |
| | FEDformer | 5.161 | 0.380 | 6.156 | 0.425 | 1.487 | | | 5.161 | 0.380 | 6.156 | 0.425 | 1.487 | | | |
| | Informer | 1.699 | 0.431 | 1.864 | 0.475 | 1.331 | | | 1.699 | 0.431 | 1.864 | 0.475 | 1.331 | | | |
| | PatchTST | 4.549 | 0.417 | 4.990 | 0.469 | 2.686 | | | 4.549 | 0.417 | 4.990 | 0.469 | 2.686 | | | |
| | Transformer | 1.390 | 0.447 | 1.652 | 0.488 | 1.506 | | | 1.390 | 0.447 | 1.652 | 0.488 | 1.506 | | | |
| | | 2.908 | 0.429 | 3.943 | 0.481 | 3.057 | | | 2.908 | 0.429 | 3.943 | 0.481 | 3.057 | | | |
| Transformer | Crossformer | 0.580 | 0.209 | 0.730 | 0.297 | 0.371 | | | 0.580 | 0.209 | 0.730 | 0.297 | 0.371 | | | |
| | FEDformer | 0.569 | 0.091 | 0.841 | 0.169 | 0.261 | | | 0.569 | 0.091 | 0.841 | 0.169 | 0.261 | | | |
| | Informer | 0.783 | 0.300 | 0.866 | 0.383 | 0.522 | | | 0.783 | 0.300 | 0.866 | 0.383 | 0.522 | | | |
| | PatchTST | 1.046 | 0.179 | 1.158 | 0.277 | 0.485 | | | 1.046 | 0.179 | 1.158 | 0.277 | 0.485 | | | |
| | Transformer | 1.045 | 0.411 | 1.077 | 0.488 | 0.882 | | | 1.045 | 0.411 | 1.077 | 0.488 | 0.882 | | | |
| | | 1.742 | 0.322 | 1.840 | 0.440 | 1.262 | | | 1.742 | 0.322 | 1.840 | 0.440 | 1.262 | | | |

Continued on next page

| | dataset | ECL | | | | ETTh1 | | | | ETTh2 | | | | Exchange | | | |
|-----------------------------------|-------------|-------------------|-------|-------|-------|-------------------|-------|-------|-------|-------------------|-------|-------|-------|-------------------|-------|-------|-------|
| | | prediction length | | | | prediction length | | | | prediction length | | | | prediction length | | | |
| | | metric | | | | metric | | | | metric | | | | metric | | | |
| UnitNorm (k=0.5) | Crossformer | 0.420 | 0.274 | 0.463 | 0.320 | 0.257 | 0.420 | 0.274 | 0.463 | 0.320 | 0.257 | 0.420 | 0.274 | 0.463 | 0.320 | 0.257 | 0.420 |
| | FEDformer | 0.331 | 0.183 | 0.401 | 0.204 | 0.156 | 0.331 | 0.183 | 0.401 | 0.204 | 0.156 | 0.331 | 0.183 | 0.401 | 0.204 | 0.156 | 0.331 |
| | Informer | 0.446 | 0.280 | 0.492 | 0.335 | 0.274 | 0.446 | 0.280 | 0.492 | 0.335 | 0.274 | 0.446 | 0.280 | 0.492 | 0.335 | 0.274 | 0.446 |
| | PatchTST | 0.371 | 0.189 | 0.434 | 0.222 | 0.176 | 0.371 | 0.189 | 0.434 | 0.222 | 0.176 | 0.371 | 0.189 | 0.434 | 0.222 | 0.176 | 0.371 |
| | Transformer | 0.504 | 0.296 | 0.501 | 0.354 | 0.299 | 0.504 | 0.296 | 0.501 | 0.354 | 0.299 | 0.504 | 0.296 | 0.501 | 0.354 | 0.299 | 0.504 |
| | Transformer | 0.460 | 0.205 | 0.441 | 0.242 | 0.204 | 0.460 | 0.205 | 0.441 | 0.242 | 0.204 | 0.460 | 0.205 | 0.441 | 0.242 | 0.204 | 0.460 |
| UnitNorm (k=1.0) | Crossformer | 0.508 | 0.328 | 0.558 | 0.385 | 0.339 | 0.508 | 0.328 | 0.558 | 0.385 | 0.339 | 0.508 | 0.328 | 0.558 | 0.385 | 0.339 | 0.508 |
| | FEDformer | 0.459 | 0.247 | 0.543 | 0.283 | 0.251 | 0.459 | 0.247 | 0.543 | 0.283 | 0.251 | 0.459 | 0.247 | 0.543 | 0.283 | 0.251 | 0.459 |
| | Informer | 0.662 | 0.397 | 0.748 | 0.428 | 0.436 | 0.662 | 0.397 | 0.748 | 0.428 | 0.436 | 0.662 | 0.397 | 0.748 | 0.428 | 0.436 | 0.662 |
| | PatchTST | 0.751 | 0.381 | 0.963 | 0.386 | 0.408 | 0.751 | 0.381 | 0.963 | 0.386 | 0.408 | 0.751 | 0.381 | 0.963 | 0.386 | 0.408 | 0.751 |
| | Transformer | 0.736 | 0.428 | 0.751 | 0.448 | 0.498 | 0.736 | 0.428 | 0.751 | 0.448 | 0.498 | 0.736 | 0.428 | 0.751 | 0.448 | 0.498 | 0.736 |
| | Transformer | 0.917 | 0.427 | 0.981 | 0.423 | 0.499 | 0.917 | 0.427 | 0.981 | 0.423 | 0.499 | 0.917 | 0.427 | 0.981 | 0.423 | 0.499 | 0.917 |
| UnitNorm (learnable; k=0.0) | Crossformer | 0.821 | 0.451 | 0.800 | 0.471 | 0.600 | 0.821 | 0.451 | 0.800 | 0.471 | 0.600 | 0.821 | 0.451 | 0.800 | 0.471 | 0.600 | 0.821 |
| | FEDformer | 1.073 | 0.466 | 1.061 | 0.462 | 0.643 | 1.073 | 0.466 | 1.061 | 0.462 | 0.643 | 1.073 | 0.466 | 1.061 | 0.462 | 0.643 | 1.073 |
| | Informer | 0.874 | 0.484 | 0.871 | 0.502 | 0.673 | 0.874 | 0.484 | 0.871 | 0.502 | 0.673 | 0.874 | 0.484 | 0.871 | 0.502 | 0.673 | 0.874 |
| | PatchTST | 1.186 | 0.493 | 1.190 | 0.497 | 0.759 | 1.186 | 0.493 | 1.190 | 0.497 | 0.759 | 1.186 | 0.493 | 1.190 | 0.497 | 0.759 | 1.186 |
| | Transformer | 0.914 | 0.343 | 1.099 | 0.401 | 0.657 | 0.914 | 0.343 | 1.099 | 0.401 | 0.657 | 0.914 | 0.343 | 1.099 | 0.401 | 0.657 | 0.914 |
| | Transformer | 1.243 | 0.291 | 1.884 | 0.356 | 0.863 | 1.243 | 0.291 | 1.884 | 0.356 | 0.863 | 1.243 | 0.291 | 1.884 | 0.356 | 0.863 | 1.243 |
| UnitNorm (learnable; k=0.7) | Crossformer | 1.391 | 0.393 | 1.410 | 0.438 | 0.832 | 1.391 | 0.393 | 1.410 | 0.438 | 0.832 | 1.391 | 0.393 | 1.410 | 0.438 | 0.832 | 1.391 |
| | FEDformer | 3.050 | 0.365 | 3.014 | 0.427 | 1.326 | 3.050 | 0.365 | 3.014 | 0.427 | 1.326 | 3.050 | 0.365 | 3.014 | 0.427 | 1.326 | 3.050 |
| | Informer | 1.356 | 0.433 | 1.343 | 0.480 | 1.120 | 1.356 | 0.433 | 1.343 | 0.480 | 1.120 | 1.356 | 0.433 | 1.343 | 0.480 | 1.120 | 1.356 |
| | PatchTST | 2.854 | 0.420 | 2.696 | 0.475 | 2.004 | 2.854 | 0.420 | 2.696 | 0.475 | 2.004 | 2.854 | 0.420 | 2.696 | 0.475 | 2.004 | 2.854 |
| | Transformer | 1.379 | 0.449 | 1.448 | 0.483 | 1.369 | 1.379 | 0.449 | 1.448 | 0.483 | 1.369 | 1.379 | 0.449 | 1.448 | 0.483 | 1.369 | 1.379 |
| | Transformer | 2.669 | 0.431 | 2.927 | 0.474 | 2.851 | 2.669 | 0.431 | 2.927 | 0.474 | 2.851 | 2.669 | 0.431 | 2.927 | 0.474 | 2.851 | 2.669 |
| UnitNorm (learnable; k=1.0) | Crossformer | 0.782 | 0.202 | 0.838 | 0.298 | 0.472 | 0.782 | 0.202 | 0.838 | 0.298 | 0.472 | 0.782 | 0.202 | 0.838 | 0.298 | 0.472 | 0.782 |
| | FEDformer | 0.965 | 0.085 | 1.068 | 0.170 | 0.430 | 0.965 | 0.085 | 1.068 | 0.170 | 0.430 | 0.965 | 0.085 | 1.068 | 0.170 | 0.430 | 0.965 |
| | Informer | 0.915 | 0.300 | 0.983 | 0.385 | 0.644 | 0.915 | 0.300 | 0.983 | 0.385 | 0.644 | 0.915 | 0.300 | 0.983 | 0.385 | 0.644 | 0.915 |
| | PatchTST | 1.328 | 0.178 | 1.457 | 0.279 | 0.702 | 1.328 | 0.178 | 1.457 | 0.279 | 0.702 | 1.328 | 0.178 | 1.457 | 0.279 | 0.702 | 1.328 |
| | Transformer | 0.993 | 0.411 | 1.028 | 0.487 | 0.964 | 0.993 | 0.411 | 1.028 | 0.487 | 0.964 | 0.993 | 0.411 | 1.028 | 0.487 | 0.964 | 0.993 |
| | Transformer | 1.484 | 0.321 | 1.595 | 0.438 | 1.526 | 1.484 | 0.321 | 1.595 | 0.438 | 1.526 | 1.484 | 0.321 | 1.595 | 0.438 | 1.526 | 1.484 |
| UnitNorm (learnable; k=0.5) | Crossformer | 0.911 | 0.698 | 1.023 | 0.820 | 1.128 | 0.911 | 0.698 | 1.023 | 0.820 | 1.128 | 0.911 | 0.698 | 1.023 | 0.820 | 1.128 | 0.911 |
| | FEDformer | 1.196 | 0.861 | 1.608 | 1.145 | 1.971 | 1.196 | 0.861 | 1.608 | 1.145 | 1.971 | 1.196 | 0.861 | 1.608 | 1.145 | 1.971 | 1.196 |
| | Informer | 0.782 | 0.202 | 0.838 | 0.298 | 0.472 | 0.782 | 0.202 | 0.838 | 0.298 | 0.472 | 0.782 | 0.202 | 0.838 | 0.298 | 0.472 | 0.782 |
| | PatchTST | 0.965 | 0.085 | 1.068 | 0.170 | 0.430 | 0.965 | 0.085 | 1.068 | 0.170 | 0.430 | 0.965 | 0.085 | 1.068 | 0.170 | 0.430 | 0.965 |
| | Transformer | 0.915 | 0.300 | 0.983 | 0.385 | 0.644 | 0.915 | 0.300 | 0.983 | 0.385 | 0.644 | 0.915 | 0.300 | 0.983 | 0.385 | 0.644 | 0.915 |
| | Transformer | 1.328 | 0.178 | 1.457 | 0.279 | 0.702 | 1.328 | 0.178 | 1.457 | 0.279 | 0.702 | 1.328 | 0.178 | 1.457 | 0.279 | 0.702 | 1.328 |
| UnitNorm (learnable; k=0.0) | Crossformer | 0.580 | 0.209 | 0.750 | 0.297 | 0.373 | 0.580 | 0.209 | 0.750 | 0.297 | 0.373 | 0.580 | 0.209 | 0.750 | 0.297 | 0.373 | 0.580 |
| | FEDformer | 0.569 | 0.091 | 0.877 | 0.169 | 0.263 | 0.569 | 0.091 | 0.877 | 0.169 | 0.263 | 0.569 | 0.091 | 0.877 | 0.169 | 0.263 | 0.569 |
| | Informer | 0.783 | 0.300 | 0.860 | 0.383 | 0.522 | 0.783 | 0.300 | 0.860 | 0.383 | 0.522 | 0.783 | 0.300 | 0.860 | 0.383 | 0.522 | 0.783 |
| | PatchTST | 1.046 | 0.179 | 1.137 | 0.277 | 0.486 | 1.046 | 0.179 | 1.137 | 0.277 | 0.486 | 1.046 | 0.179 | 1.137 | 0.277 | 0.486 | 1.046 |
| | Transformer | 1.046 | 0.411 | 1.077 | 0.488 | 0.886 | 1.046 | 0.411 | 1.077 | 0.488 | 0.886 | 1.046 | 0.411 | 1.077 | 0.488 | 0.886 | 1.046 |
| | Transformer | 1.742 | 0.322 | 1.841 | 0.440 | 1.270 | 1.742 | 0.322 | 1.841 | 0.440 | 1.270 | 1.742 | 0.322 | 1.841 | 0.440 | 1.270 | 1.742 |
| UnitNorm (learnable; k=0.7) | Crossformer | 1.246 | 0.715 | 1.396 | 0.824 | 1.048 | 1.246 | 0.715 | 1.396 | 0.824 | 1.048 | 1.246 | 0.715 | 1.396 | 0.824 | 1.048 | 1.246 |
| | FEDformer | 2.354 | 0.904 | 2.936 | 1.153 | 1.702 | 2.354 | 0.904 | 2.936 | 1.153 | 1.702 | 2.354 | 0.904 | 2.936 | 1.153 | 1.702 | 2.354 |
| | Informer | 0.580 | 0.209 | 0.750 | 0.297 | 0.373 | 0.580 | 0.209 | 0.750 | 0.297 | 0.373 | 0.580 | 0.209 | 0.750 | 0.297 | 0.373 | 0.580 |
| | PatchTST | 0.569 | 0.091 | 0.877 | 0.169 | 0.263 | 0.569 | 0.091 | 0.877 | 0.169 | 0.263 | 0.569 | 0.091 | 0.877 | 0.169 | 0.263 | 0.569 |
| | Transformer | 0.783 | 0.300 | 0.860 | 0.383 | 0.522 | 0.783 | 0.300 | 0.860 | 0.383 | 0.522 | 0.783 | 0.300 | 0.860 | 0.383 | 0.522 | 0.783 |
| | Transformer | 1.046 | 0.179 | 1.137 | 0.277 | 0.486 | 1.046 | 0.179 | 1.137 | 0.277 | 0.486 | 1.046 | 0.179 | 1.137 | 0.277 | 0.486 | 1.046 |
| UnitNorm (learnable; k=1.0) | Crossformer | 0.985 | 0.341 | 1.093 | 0.396 | 0.568 | 0.985 | 0.341 | 1.093 | 0.396 | 0.568 | 0.985 | 0.341 | 1.093 | 0.396 | 0.568 | 0.985 |
| | FEDformer | 1.495 | 0.290 | 1.861 | 0.355 | 0.673 | 1.495 | 0.290 | 1.861 | 0.355 | 0.673 | 1.495 | 0.290 | 1.861 | 0.355 | 0.673 | 1.495 |
| | Informer | 1.160 | 0.394 | 1.251 | 0.445 | 0.797 | 1.160 | 0.394 | 1.251 | 0.445 | 0.797 | 1.160 | 0.394 | 1.251 | 0.445 | 0.797 | 1.160 |
| | PatchTST | 2.112 | 0.369 | 2.407 | 0.434 | 1.268 | 2.112 | 0.369 | 2.407 | 0.434 | 1.268 | 2.112 | 0.369 | 2.407 | 0.434 | 1.268 | 2.112 |
| | Transformer | 1.229 | 0.429 | 1.268 | 0.480 | 0.834 | 1.229 | 0.429 | 1.268 | 0.480 | 0.834 | 1.229 | 0.429 | 1.268 | 0.480 | 0.834 | 1.229 |
| | Transformer | 2.378 | 0.417 | 2.314 | 0.475 | 1.379 | 2.378 | 0.417 | 2.314 | 0.475 | 1.379 | 2.378 | 0.417 | 2.314 | 0.475 | 1.379 | 2.378 |
| UnitNorm (learnable; k=0.5) | Crossformer | 1.290 | 0.449 | 1.305 | 0.485 | 1.041 | 1.290 | 0.449 | 1.305 | 0.485 | 1.041 | 1.290 | 0.449 | 1.305 | 0.485 | 1.041 | 1.290 |
| | FEDformer | 2.399 | 0.429 | 2.436 | 0.480 | 1.914 | 2.399 | 0.429 | 2.436 | 0.480 | 1.914 | 2.399 | 0.429 | 2.436 | 0.480 | 1.914 | 2.399 |
| | Informer | 1.023 | 0.202 | 1.031 | 0.293 | 0.688 | 1.023 | 0.202 | 1.031 | 0.293 | 0.688 | 1.023 | 0.202 | 1.031 | 0.293 | 0.688 | 1.023 |
| | PatchTST | 1.535 | 0.084 | 1.527 | 0.164 | 0.913 | 1.535 | 0.084 | 1.527 | 0.164 | 0.913 | 1.535 | 0.084 | 1.527 | 0.164 | 0.913 | 1.535 |
| | Transformer | 1.121 | 0.300 | 1.075 | 0.385 | 0.772 | 1.121 | 0.300 | 1.075 | 0.385 | 0.772 | 1.121 | 0.300 | 1.075 | 0.385 | 0.772 | 1.121 |
| | Transformer | 1.848 | 0.180 | 1.725 | 0.280 | 1.057 | 1.848 | 0.180 | 1.725 | 0.280 | 1.057 | 1.848 | 0.180 | 1.725 | 0.280 | 1.057 | 1.848 |
| UnitNorm (learnable; k=0.0) | Crossformer | 1.203 | 0.418 | 1.186 | 0.487 | 1.177 | 1.203 | 0.418 | 1.186 | 0.487 | 1.177 | 1.203 | 0.418 | 1.186 | 0.487 | 1.177 | 1.203 |
| | FEDformer | 2.122 | 0.331 | 2.042 | 0.438 | 2.187 | 2.122 | 0.331 | 2.042 | 0.438 | 2.187 | 2.122 | 0.331 | 2.042 | 0.438 | 2.187 | 2.122 |
| | Informer | 1.111 | 0.703 | 1.163 | 0.830 | 1.338 | 1.111 | 0.703 | 1.163 | 0.830 | 1.338 | 1.111 | 0.703 | 1.163 | 0.830 | 1.338 | 1.111 |
| | PatchTST | 1.717 | 0.869 | 2.031 | 1.167 | 2.711 | 1.717 | 0.869 | 2.031 | 1.167 | 2.711 | 1.717 | 0.869 | 2.031 | 1.167 | 2.711 | |

Table S7: Classification accuracies of different datasets using different models and normalization methods. For each dataset and for each model, the best performing normalization method(s) are bolded, and the second best are underlined.

| | dataset | Face Detection | Heartbeat | PEMS-SF | UWave Gesture Library |
|-----------------------------------|-------------|-------------------|---------------|---------------|-----------------------------|
| BatchNorm | Crossformer | 50.435 | 75.122 | 68.401 | 83.438 |
| | FEDformer | 68.275 | <u>73.984</u> | 78.035 | 47.812 |
| | Informer | 68.606 | 73.984 | 87.476 | 82.083 |
| | PatchTST | 65.683 | 66.992 | 79.576 | 81.354 |
| | Transformer | 68.663 | <u>75.610</u> | <u>84.200</u> | 83.542 |
| LayerNorm | Crossformer | 52.176 | 73.008 | 26.397 | <u>82.708</u> |
| | FEDformer | <u>68.861</u> | 73.659 | 84.393 | <u>48.438</u> |
| | Informer | 68.076 | 73.821 | <u>85.742</u> | 81.979 |
| | PatchTST | 67.329 | 69.919 | 84.971 | 81.562 |
| | Transformer | <u>68.757</u> | 74.472 | 82.466 | <u>85.104</u> |
| RMSNORM | Crossformer | <u>51.693</u> | <u>73.659</u> | 23.699 | 81.042 |
| | FEDformer | 68.000 | <u>72.846</u> | <u>85.164</u> | 47.708 |
| | Informer | 68.275 | <u>75.447</u> | 84.586 | 83.125 |
| | PatchTST | 66.648 | 70.894 | 82.852 | 80.729 |
| | Transformer | 69.154 | 75.935 | 83.237 | 84.167 |
| UnitNorm (k=0.0) | Crossformer | 50.000 | 72.195 | 16.763 | 29.167 |
| | FEDformer | 69.041 | 74.146 | 83.430 | 53.333 |
| | Informer | 69.088 | 75.285 | 78.035 | 85.000 |
| | PatchTST | <u>67.546</u> | 72.195 | 81.118 | <u>82.396</u> |
| | Transformer | <u>68.568</u> | 75.935 | 82.659 | 87.188 |
| UnitNorm (k=0.7) | Crossformer | 50.236 | 73.008 | <u>65.896</u> | 81.667 |
| | FEDformer | 68.067 | 72.846 | 84.586 | 47.083 |
| | Informer | 68.142 | 72.846 | 83.237 | <u>83.958</u> |
| | PatchTST | 67.641 | <u>72.358</u> | 84.971 | 82.604 |
| | Transformer | 68.634 | 74.797 | 84.200 | 84.896 |
| UnitNorm (k=1.0) | Crossformer | 50.019 | 72.195 | 56.455 | 80.521 |
| | FEDformer | 67.357 | <u>73.984</u> | 85.356 | 48.125 |
| | Informer | 68.492 | 73.984 | 84.008 | 83.646 |
| | PatchTST | 67.452 | 72.033 | <u>83.044</u> | 81.146 |
| | Transformer | 68.350 | 73.984 | 80.347 | 84.375 |
| UnitNorm (learnable; k=0.0) | Crossformer | 50.000 | 72.195 | 16.763 | 29.167 |
| | FEDformer | 69.041 | 74.146 | 83.430 | 53.333 |
| | Informer | <u>69.079</u> | 74.959 | 80.539 | 85.000 |
| | PatchTST | <u>67.546</u> | 72.195 | 81.118 | <u>82.396</u> |
| | Transformer | 68.568 | 75.935 | 82.659 | 87.188 |
| UnitNorm (learnable; k=0.7) | Crossformer | 50.000 | 72.195 | 16.763 | 29.167 |
| | FEDformer | 69.041 | 74.146 | 83.430 | 53.333 |
| | Informer | 68.852 | 75.122 | 78.420 | 85.000 |
| | PatchTST | <u>67.546</u> | 72.195 | 81.118 | <u>82.396</u> |
| | Transformer | 68.568 | 75.935 | 82.659 | 87.188 |
| UnitNorm (learnable; k=1.0) | Crossformer | 50.000 | 72.195 | 16.763 | 29.167 |
| | FEDformer | 69.041 | 74.146 | 83.430 | 53.333 |
| | Informer | 68.558 | 75.610 | 79.576 | 85.000 |
| | PatchTST | <u>67.546</u> | 72.846 | 81.118 | <u>82.396</u> |
| | Transformer | 68.568 | 75.935 | 82.659 | 87.188 |

Table S8: Anomaly detection accuracies of MSL dataset using different models and normalization methods. For each metric and for each model, the best performing normalization method(s) are bolded, and the second best are underlined.

| | metric | Accuracy | F-score | Precision | Recall |
|-----------------------------------|-------------|---------------|---------------|---------------|---------------|
| BatchNorm | Crossformer | 93.507 | 59.110 | 81.410 | 47.903 |
| | FEDformer | 95.543 | 75.820 | 88.630 | 66.240 |
| | Informer | 93.040 | 56.927 | 81.760 | 43.733 |
| | PatchTST | 95.947 | 78.613 | 88.603 | 70.650 |
| | Transformer | 90.417 | 30.680 | 64.623 | 20.123 |
| LayerNorm | Crossformer | 96.313 | 80.640 | 90.330 | 72.823 |
| | FEDformer | 96.603 | 82.427 | 90.697 | 75.537 |
| | Informer | 96.390 | 81.193 | 90.120 | 73.877 |
| | PatchTST | 95.950 | 78.727 | 88.347 | 70.993 |
| | Transformer | 96.333 | 80.910 | 89.740 | 73.660 |
| RMSNorm | Crossformer | 96.307 | 80.613 | 90.323 | 72.790 |
| | FEDformer | 96.573 | 82.263 | 90.647 | 75.300 |
| | Informer | 96.373 | 81.067 | 90.097 | 73.680 |
| | PatchTST | 95.940 | 78.670 | 88.307 | 70.927 |
| | Transformer | 96.330 | 80.883 | 89.677 | 73.657 |
| UnitNorm (k=0.0) | Crossformer | 96.533 | 82.000 | <u>90.610</u> | 74.880 |
| | FEDformer | 96.547 | 82.097 | 90.653 | 75.013 |
| | Informer | <u>96.543</u> | <u>82.067</u> | <u>90.640</u> | <u>74.973</u> |
| | PatchTST | 96.317 | 80.943 | 88.990 | 74.227 |
| | Transformer | <u>96.540</u> | 82.060 | 90.637 | 74.960 |
| UnitNorm (k=0.7) | Crossformer | <u>96.523</u> | <u>81.943</u> | 90.617 | <u>74.783</u> |
| | FEDformer | 96.537 | 82.040 | 90.620 | 74.943 |
| | Informer | 96.557 | 82.147 | 90.643 | 75.103 |
| | PatchTST | <u>96.213</u> | <u>80.360</u> | <u>88.713</u> | <u>73.440</u> |
| | Transformer | 96.540 | 82.043 | <u>90.580</u> | <u>74.977</u> |
| UnitNorm (k=1.0) | Crossformer | 96.347 | 80.857 | 90.380 | 73.143 |
| | FEDformer | <u>96.587</u> | <u>82.350</u> | <u>90.670</u> | <u>75.433</u> |
| | Informer | 96.470 | 81.653 | 90.400 | 74.450 |
| | PatchTST | 95.933 | 78.607 | 88.273 | 70.847 |
| | Transformer | 96.337 | <u>80.933</u> | 89.753 | 73.687 |
| UnitNorm (learnable; k=0.0) | Crossformer | 96.533 | 82.000 | <u>90.610</u> | 74.880 |
| | FEDformer | 96.547 | 82.097 | 90.653 | 75.013 |
| | Informer | <u>96.543</u> | <u>82.067</u> | <u>90.640</u> | <u>74.973</u> |
| | PatchTST | 96.317 | 80.943 | 88.990 | 74.227 |
| | Transformer | <u>96.540</u> | 82.060 | 90.637 | 74.960 |
| UnitNorm (learnable; k=0.7) | Crossformer | 96.533 | 82.000 | <u>90.610</u> | 74.880 |
| | FEDformer | 96.547 | 82.097 | 90.653 | 75.013 |
| | Informer | <u>96.543</u> | <u>82.067</u> | <u>90.640</u> | <u>74.973</u> |
| | PatchTST | 96.317 | 80.943 | 88.990 | 74.227 |
| | Transformer | <u>96.540</u> | 82.060 | 90.637 | 74.960 |
| UnitNorm (learnable; k=1.0) | Crossformer | 96.533 | 82.000 | <u>90.610</u> | 74.880 |
| | FEDformer | 96.547 | 82.097 | 90.653 | 75.013 |
| | Informer | <u>96.543</u> | <u>82.067</u> | <u>90.640</u> | <u>74.973</u> |
| | PatchTST | 96.317 | 80.943 | 88.990 | 74.227 |
| | Transformer | <u>96.540</u> | 82.060 | 90.637 | 74.960 |

Table S9: Metrics used for characterizing the distribution of attention scores from the original and normalized data, denoted as $\mathbf{A}_{n,i}$ and $\tilde{\mathbf{A}}_{n,i}$, respectively, for the i -th sample in the n -th batch.

| Metric | Definition | Evaluation |
|--------------------|---|------------------|
| Chebyshev distance | $D_{\text{Chebyshev}}(\mathbf{A}_{n,i}, \tilde{\mathbf{A}}_{n,i}) = \max_{j=1}^L \left \mathbf{A}_{n,i,j} - \tilde{\mathbf{A}}_{n,i,j} \right $ | Lower is Better |
| Cosine similarity | $D_{\text{Cosine}}(\mathbf{A}_{n,i}, \tilde{\mathbf{A}}_{n,i}) = \frac{\mathbf{A}_{n,i}^\top \tilde{\mathbf{A}}_{n,i}}{\ \mathbf{A}_{n,i}\ \ \tilde{\mathbf{A}}_{n,i}\ }$ | Higher is Better |
| KL divergence | $D_{\text{KL}}(\mathbf{A}_{n,i} \parallel \tilde{\mathbf{A}}_{n,i}) = \sum_{j=1}^L \mathbf{A}_{n,i,j} \left(\log \mathbf{A}_{n,i,j} - \log \tilde{\mathbf{A}}_{n,i,j} \right)$ | Lower is Better |
| Entropy | $E(\tilde{\mathbf{A}}_{n,i}) = - \sum_{j=1}^L \tilde{\mathbf{A}}_{n,i,j} \log \tilde{\mathbf{A}}_{n,i,j}$ | Higher is Better |

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