SortFormer: Permutation Encoding for Transformer

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Abstract

We propose SortFormer architecture, which is a Transformer variant that encodes permutation information into hidden states. We address the challenge of permutation invariance in processing sequential data using Transformer architectures. Despite their effectiveness in learning and generalizing across text, speech, and image data, Transformers struggle with inputs where permutations should be disregarded. This limitation often results in significant overfitting where the trained model hardly handles permutations on on the unseen datapoints. We identify that the inherent design of the original Transformer architecture contributes to this deficiency. SortFormer operates by generating estimated labels at each layer, which are then sorted according to their arrival order. These sequentially ordered labels serve as a permutative encoding, guiding the Transformer model in recognizing the sequence order. Through ablation studies, we demonstrate that SortFormer exhibits reduced overfitting and enhanced generalization capabilities on unseen data sequences. Furthermore, we provide insights into the practical applicability of SortFormer in real-world scenarios. Our findings suggest that this innovative architecture holds significant promise for improving the robustness and versatility of Transformer models in handling permutation-sensitive sequential data.

1 Introduction

Testing autobuild 7

In recent years, the large language models (LLMs) [12, 15] gained significant popularity and most of the LLMs are based on the Transformer [17] architecture that is now being used for not only language modeling as language understanding [6, 14], GPT3 [3]. Other tasks such as image processing field also started leveraging Transformers such as image generation [11] and image recognition with ViT [7]. In speech recognition field, Conformer [8] and Whisper [13] successfully employed Transformer architecture to speech-to-text (STT) tasks.

Transformer Variants for Efficiency The wide adoption of Transformer architecture also led to more efficient variants of the model such as Reformer [9], which introduces efficient memory handling in Transformers through locality-sensitive hashing; Transformer-XL [5], enhancing Transformer models for long sequence tasks with segment-level recurrence and a novel positional encoding; Performe [4], offering a scalable Transformer variant with the new attention mechanism for processing long sequences efficiently; Longformer [1], designed for longer texts with a modified attention mechanism that combines sliding window and global attention for tasks like document classification and question answering; SegFormer [18], an approach for semantic segmentation combining a hierarchical Transformer encoder with a lightweight MLP decoder; and RoFormer[16], which enhances Transformer models with a rotational position encoding scheme for improved performance in various natural language processing tasks. These variants showcase significant advancements in handling

^{*}Use footnote for providing further information about author (webpage, alternative address)—not for acknowledging funding agencies.

long sequences, improving memory efficiency, and extending the applicability of Transformer models in various domains, including text and image processing.

Problem that SortFormer solves The input sequence X can be represented as:

$$\mathbf{X} = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_T\} \tag{1}$$

$$\mathbf{Y} = \{\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_T\} \tag{2}$$

where each x_i is a vector representing a token or embedding in the input sequence.

The output sequence Y can be represented as:

where each y_i is a vector representing a token in the output sequence.

We propose a model designed for the simultaneous estimation of class presences from a sequence of input tokens. Consider a set of frame-wise F-dimensional embedding vectors $\{\mathbf{x}_t\}_{t=1}^T$, where $\mathbf{x}_t \in \mathbb{R}^D, t=1,2,\ldots,T$, representing the frame index. SortFormer is tasked with estimating the class presences $(\mathbf{y}_t)_{t=1}^T$. In this context, $\mathbf{y}_t = [y_{1,t}, y_{2,t}, \ldots, y_{K,t}]^{\mathsf{T}}$ denotes the class presences of K classes at time t. Each $y_{k,t}$ is defined as follows:

$$y_{k,t} = \begin{cases} 0, & \text{if class } k \text{ is present at time } t, \\ 1, & \text{if class } k \text{ is not present at time } t. \end{cases}$$
 (3)

SortFormer operates under the assumption that $y_{k,t}$ is conditionally independent given the embedding vectors (features). This assumption is formalized as:

$$P(\mathbf{y}_1, \dots, \mathbf{y}_T \mid \mathbf{x}_1, \dots, \mathbf{x}_T) = \prod_{k=1}^K \prod_{t=1}^T P(y_{k,t} \mid \mathbf{x}_1, \dots, \mathbf{x}_T).$$
(4)

Under this framework, the task at hand is construed as a multi-label classification problem, which is amenable to modeling via a neural network, denoted as f_{Θ} . The model is defined as:

$$(\mathbf{p}_1, \dots, \mathbf{p}_T) = f_{\Theta}(\mathbf{x}_1, \dots, \mathbf{x}_T), \tag{5}$$

where $\mathbf{p}_t = [p_{1,t},\dots,p_{K,t}]^{\top} \in (0,1)^S$ represents the posterior probabilities of the presences of S classes at frame index t and f represents the Sortformer model with parameter . The estimation of speech presences $\{\hat{\mathbf{y}}_t\}_{t=1}^T$ is given by:

$$\hat{\mathbf{y}}_{1}, \dots, \hat{\mathbf{y}}_{T} = \underset{\mathbf{y}_{k} \in \mathbf{Y}}{\operatorname{arg max}} P\left(\mathbf{y}_{1}, \dots, \mathbf{y}_{T} \mid \mathbf{x}_{1}, \dots, \mathbf{x}_{T}\right),$$
(6)

Permutation Invariance in Neural Network Problem

2 Prior Works

clustering There have been numerous studies on making Transformer to perceive longer context, model compressing for memory efficiency and sparse models. However, there have been limited number of published work regarding general-purpose transformer variants which can handle permutation

The most closest previous study to our work is Set-Transformer [10],

permutation invairant loss

clustering

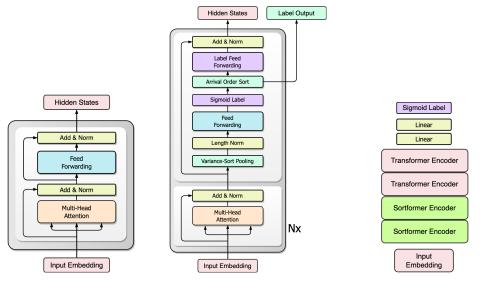


Figure 1: Caption1

Figure 2: Caption 2

Figure 3: Caption 3

3 Permutation Invariance for Transformers

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[2]. This section is fo Let $Y \in \mathcal{Y}$ be some random variable of interest, to be predicted from \mathbf{X}_n . Permutation invariance of the conditional distribution $P_{Y|\mathbf{x}_n}$ of Y given \mathbf{X}_n is defined as follows.

Definition 1. The conditional distribution $P_{Y|\mathbf{X}_n}$ of Y given \mathbf{X}_n is \mathbb{S}_n -invariant if for all $B \in \mathcal{B}(\mathcal{Y})$ and $\pi \in \mathbb{S}_n$,

$$P_{Y\mid\mathbf{X}_n}\left[Y\in B\mid\pi\cdot\mathbf{X}_n\right] = P_{Y\mid\mathbf{X}_n}\left[Y\in B\mid\mathbf{X}_n\right] \quad \text{a.s. } -P_{\mathbf{X}_n}. \tag{7}$$

Together with exchangeability of $P_{\mathbf{X}_n}$, conditional invariance implies the joint equality $(\pi \cdot \mathbf{X}_n, Y) \stackrel{\mathrm{d}}{=} (\mathbf{X}_n, Y)$ for all $\pi \in \mathbb{S}_n$.

In the neural networks literature, equivariance plays a key role in the hidden layers of invariant deterministic neural networks [2,8,6]. As we show in Section 2, the following adaptation to random variables plays the same role in \mathbb{S}_n -invariant stochastic neural networks.

Definition 2. Let $\mathbf{Y}_n \in \mathcal{Y}^n$ be a random \mathcal{Y} -valued sequence. The conditional distribution $P_{\mathbf{Y}_n|\mathbf{x}_n}$ of \mathbf{Y}_n given \mathbf{X}_n is \mathbb{S}_n -equivariant if for all $B \in \mathcal{B}(\mathcal{Y}^n)$ and $\pi \in \mathbb{S}_n$,

$$P_{\mathbf{Y}_n|\mathbf{X}_n}[\pi \cdot \mathbf{Y}_n \in B \mid \pi \cdot \mathbf{X}_n] = P_{\mathbf{Y}_n|\mathbf{X}_n}[\mathbf{Y}_n \in B \mid \mathbf{X}_n] \quad \text{a.s. } -P_{\mathbf{X}_n}.$$
 (8)

Together with exchangeability of $P_{\mathbf{X}_n}$, conditional invariance implies the joint equality $(\pi \cdot \mathbf{X}_n, \pi \cdot \mathbf{Y}_n) \stackrel{\mathrm{d}}{=} (\mathbf{X}_n, \mathbf{Y}_n)$ for all $\pi \in \mathbb{S}_n$

4 Submission of papers to NeurIPS 2023

Please [17] read the instructions below carefully and follow them faithfully. **Important:** This year the checklist will be submitted separately from the main paper in OpenReview, please review it well ahead of the submission deadline: https://neurips.cc/public/guides/PaperChecklist.

4.1 Style

Papers to be submitted to NeurIPS 2023 must be prepared according to the instructions presented here. Papers may only be up to **nine** pages long, including figures. Additional pages *containing only acknowledgments and references* are allowed. Papers that exceed the page limit will not be reviewed, or in any other way considered for presentation at the conference.

The margins in 2023 are the same as those in previous years.

Authors are required to use the NeurIPS LATEX style files obtainable at the NeurIPS website as indicated below. Please make sure you use the current files and not previous versions. Tweaking the style files may be grounds for rejection.

4.2 Retrieval of style files

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The only supported style file for NeurIPS 2023 is neurips_2023.sty, rewritten for LATEX 2ε . Previous style files for LATEX 2.09, Microsoft Word, and RTF are no longer supported!

The LaTeX style file contains three optional arguments: final, which creates a camera-ready copy, preprint, which creates a preprint for submission to, e.g., arXiv, and nonatbib, which will not load the natbib package for you in case of package clash.

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The formatting instructions contained in these style files are summarized in Sections 5, 6, and 7 below.

5 General formatting instructions

The text must be confined within a rectangle 5.5 inches (33 picas) wide and 9 inches (54 picas) long. The left margin is 1.5 inch (9 picas). Use 10 point type with a vertical spacing (leading) of 11 points. Times New Roman is the preferred typeface throughout, and will be selected for you by default. Paragraphs are separated by $\frac{1}{2}$ line space (5.5 points), with no indentation.

The paper title should be 17 point, initial caps/lower case, bold, centered between two horizontal rules. The top rule should be 4 points thick and the bottom rule should be 1 point thick. Allow ¼ inch space above and below the title to rules. All pages should start at 1 inch (6 picas) from the top of the page.

For the final version, authors' names are set in boldface, and each name is centered above the corresponding address. The lead author's name is to be listed first (left-most), and the co-authors' names (if different address) are set to follow. If there is only one co-author, list both author and co-author side by side.

Please pay special attention to the instructions in Section 7 regarding figures, tables, acknowledgments, and references.

6 Headings: first level

All headings should be lower case (except for first word and proper nouns), flush left, and bold.

First-level headings should be in 12-point type.

6.1 Headings: second level

Second-level headings should be in 10-point type.

6.1.1 Headings: third level

Third-level headings should be in 10-point type.

Paragraphs There is also a \paragraph command available, which sets the heading in bold, flush left, and inline with the text, with the heading followed by 1 em of space.

7 Citations, figures, tables, references

These instructions apply to everyone.

7.1 Citations within the text

The natbib package will be loaded for you by default. Citations may be author/year or numeric, as long as you maintain internal consistency. As to the format of the references themselves, any style is acceptable as long as it is used consistently.

The documentation for natbib may be found at

```
http://mirrors.ctan.org/macros/latex/contrib/natbib/natnotes.pdf
```

Of note is the command \citet, which produces citations appropriate for use in inline text. For example,

```
\citet{hasselmo} investigated\dots
```

produces

Hasselmo, et al. (1995) investigated...

If you wish to load the natbib package with options, you may add the following before loading the neurips_2023 package:

```
\PassOptionsToPackage{options}{natbib}
```

If natbib clashes with another package you load, you can add the optional argument nonatbib when loading the style file:

```
\usepackage[nonatbib]{neurips_2023}
```

As submission is double blind, refer to your own published work in the third person. That is, use "In the previous work of Jones et al. [4]," not "In our previous work [4]." If you cite your other papers that are not widely available (e.g., a journal paper under review), use anonymous author names in the citation, e.g., an author of the form "A. Anonymous" and include a copy of the anonymized paper in the supplementary material.

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Footnotes should be used sparingly. If you do require a footnote, indicate footnotes with a number² in the text. Place the footnotes at the bottom of the page on which they appear. Precede the footnote with a horizontal rule of 2 inches (12 picas).

²Sample of the first footnote.

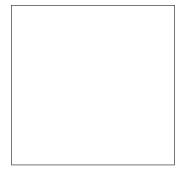


Figure 4: Sample figure caption.

Table 1: Sample table title

	Part	
Name	Description	Size (μm)
Dendrite Axon Soma	Input terminal Output terminal Cell body	$\begin{array}{c} \sim \! 100 \\ \sim \! 10 \\ \text{up to } 10^6 \end{array}$

Note that footnotes are properly typeset after punctuation marks.³

7.3 Figures

All artwork must be neat, clean, and legible. Lines should be dark enough for purposes of reproduction. The figure number and caption always appear after the figure. Place one line space before the figure caption and one line space after the figure. The figure caption should be lower case (except for first word and proper nouns); figures are numbered consecutively.

You may use color figures. However, it is best for the figure captions and the paper body to be legible if the paper is printed in either black/white or in color.

7.4 Tables

All tables must be centered, neat, clean and legible. The table number and title always appear before the table. See Table 1.

Place one line space before the table title, one line space after the table title, and one line space after the table. The table title must be lower case (except for first word and proper nouns); tables are numbered consecutively.

Note that publication-quality tables *do not contain vertical rules*. We strongly suggest the use of the booktabs package, which allows for typesetting high-quality, professional tables:

https://www.ctan.org/pkg/booktabs

This package was used to typeset Table 1.

7.5 Math

Note that display math in bare TeX commands will not create correct line numbers for submission. Please use LaTeX (or AMSTeX) commands for unnumbered display math. (You really shouldn't be using \$\$ anyway; see https://tex.stackexchange.com/questions/503/why-is-preferable-to and https://tex.stackexchange.com/questions/40492/what-are-the-differences-between-align-equation-and-displaymath for more information.)

³As in this example.

7.6 Final instructions

Do not change any aspects of the formatting parameters in the style files. In particular, do not modify the width or length of the rectangle the text should fit into, and do not change font sizes (except perhaps in the **References** section; see below). Please note that pages should be numbered.

8 Preparing PDF files

Please prepare submission files with paper size "US Letter," and not, for example, "A4."

Fonts were the main cause of problems in the past years. Your PDF file must only contain Type 1 or Embedded TrueType fonts. Here are a few instructions to achieve this.

- You should directly generate PDF files using pdflatex.
- You can check which fonts a PDF files uses. In Acrobat Reader, select the menu Files>Document Properties>Fonts and select Show All Fonts. You can also use the program pdffonts which comes with xpdf and is available out-of-the-box on most Linux machines.
- xfig "patterned" shapes are implemented with bitmap fonts. Use "solid" shapes instead.
- The \bbold package almost always uses bitmap fonts. You should use the equivalent AMS Fonts:

```
\usepackage{amsfonts}
```

followed by, e.g., \mathbb{R} , \mathbb{R} , \mathbb{R} , or \mathbb{R} , \mathbb{R} or \mathbb{R} . You can also use the following workaround for reals, natural and complex:

```
\newcommand{\RR}{I\!\!R} %real numbers
\newcommand{\Nat}{I\!\!N} %natural numbers
\newcommand{\CC}{I\!\!\!C} %complex numbers
```

Note that amsforts is automatically loaded by the amssymb package.

If your file contains type 3 fonts or non embedded TrueType fonts, we will ask you to fix it.

8.1 Margins in LATEX

Most of the margin problems come from figures positioned by hand using \special or other commands. We suggest using the command \includegraphics from the graphicx package. Always specify the figure width as a multiple of the line width as in the example below:

```
\usepackage[pdftex]{graphicx} ...
\includegraphics[width=0.8\linewidth]{myfile.pdf}
```

See Section 4.4 in the graphics bundle documentation (http://mirrors.ctan.org/macros/latex/required/graphics/grfguide.pdf)

A number of width problems arise when LATEX cannot properly hyphenate a line. Please give LaTeX hyphenation hints using the \- command when necessary.

Acknowledgments and Disclosure of Funding

Use unnumbered first level headings for the acknowledgments. All acknowledgments go at the end of the paper before the list of references. Moreover, you are required to declare funding (financial activities supporting the submitted work) and competing interests (related financial activities outside the submitted work). More information about this disclosure can be found at: https://neurips.cc/Conferences/2023/PaperInformation/FundingDisclosure.

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9 Supplementary Material

Authors may wish to optionally include extra information (complete proofs, additional experiments and plots) in the appendix. All such materials should be part of the supplemental material (submitted separately) and should NOT be included in the main submission.

References

References follow the acknowledgments in the camera-ready paper. Use unnumbered first-level heading for the references. Any choice of citation style is acceptable as long as you are consistent. It is permissible to reduce the font size to small (9 point) when listing the references. Note that the Reference section does not count towards the page limit.

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