More Identifiable yet Equally Performant Transformers for Text Classification

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Motivation

Interpretability is an important aspect when it comes to **trust** a model's prediction.

- Famous Transformer architecture-based systems are ubiquitous.
- Multi-head self-attention is its basic building block.

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Identifiability of attention weights

“Identifiable if they can be uniquely determined from the head’s output”

-On identifiability in transformers [Brunner et al., 2019]

Why is it important?

- Explanations based on them non-unique attention weights might be misleading.

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Attention Head: Phase1

Query matrix Key matrix

$$\mathbf{A} = \text{softmax}\left(\frac{\mathbf{Q}\,\mathbf{K}^T}{\sqrt{d_q}}\right)$$

d_q: size of query and key vector

Row vectors in Query and Key matrices represent token transformations.

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Dot product

(i, j) element of Attention matrix $\mathbf{A}$ denotes how much of token **i** attends to token **j.**

Attention Head: Phase2

From phase1:

$$\mathbf{A} = \mathrm{softmax}\left(\frac{\mathbf{Q}\,\mathbf{K}^T}{\sqrt{d_q}}\right)$$

$\mathbf{Q}$ and $\mathbf{K}$ are $d_s \times d_k$ matrices.
$(d_q = d_k)$

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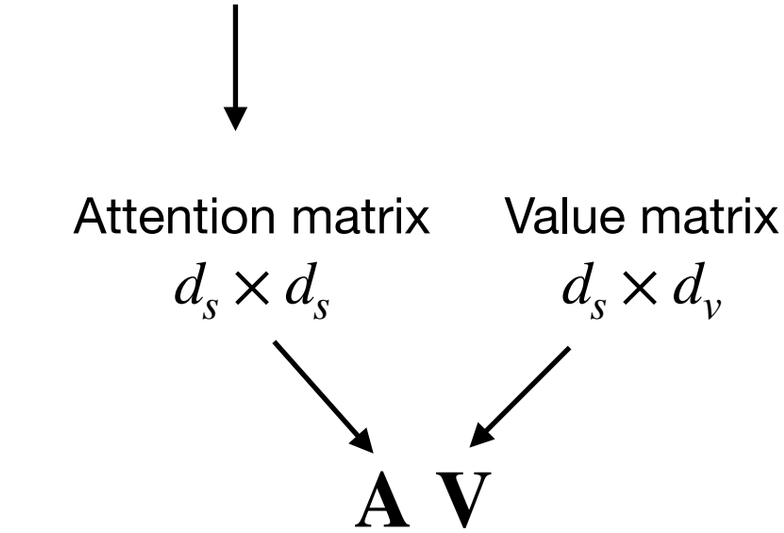

In phase2:

d_s: number of tokens

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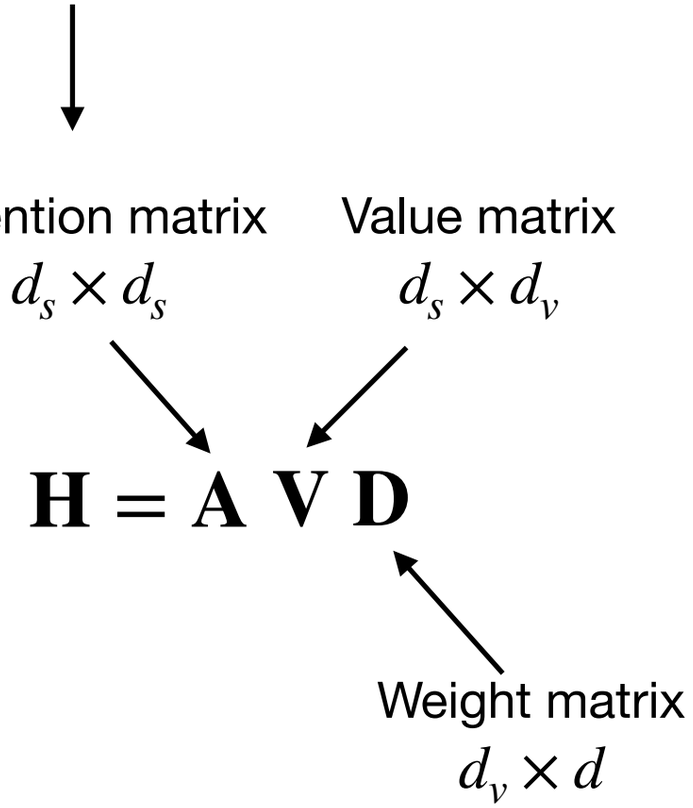

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d : size of token vector (from embedding space)

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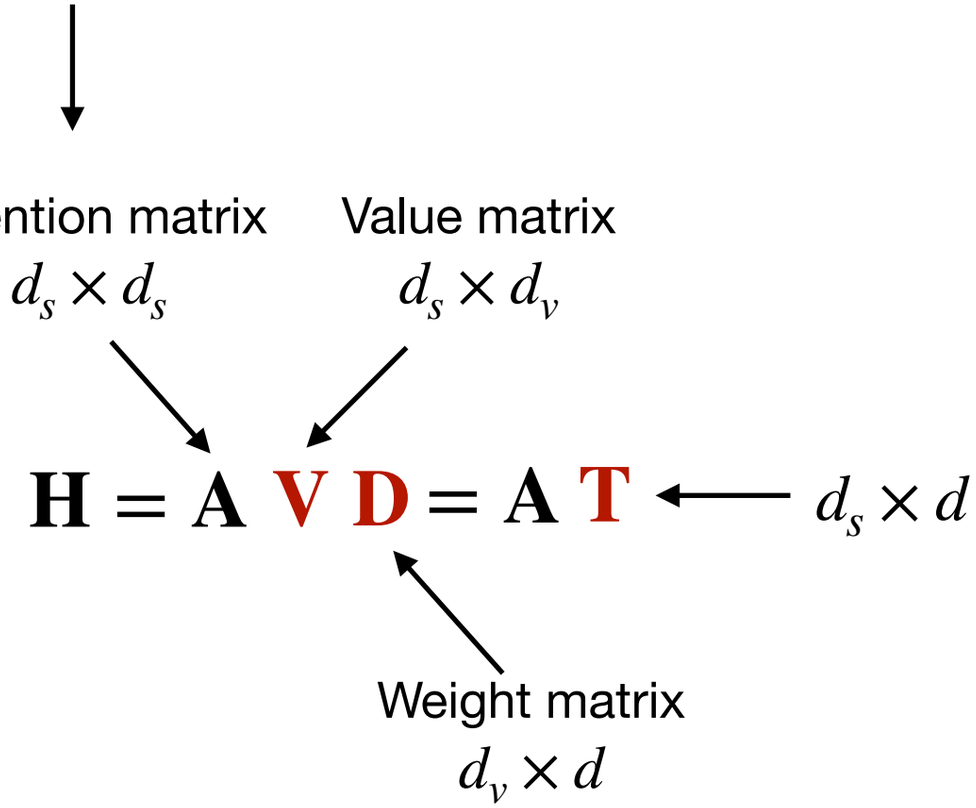

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Uniqueness of A

$$\mathbf{H} = \mathbf{A}\ \mathbf{T}$$

Is $\mathbf{A}$ unique to the combination $\mathbf{H}$ and $\mathbf{T}$?

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$$(\mathbf{A} + \tilde{\mathbf{A}})\ \mathbf{T} = \mathbf{A}\ \mathbf{T}$$
$$\Longrightarrow \tilde{\mathbf{A}}\ \mathbf{T} = \mathbf{0}$$

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Constraint-2

$$(\mathbf{A} + \tilde{\mathbf{A}})\ \mathbf{1} = \mathbf{1}$$
$$\implies \tilde{\mathbf{A}}\ \mathbf{1} = \mathbf{0}$$

Constraint-3

$$(\mathbf{A} + \tilde{\mathbf{A}}) \geq \mathbf{0}$$

probability constraints

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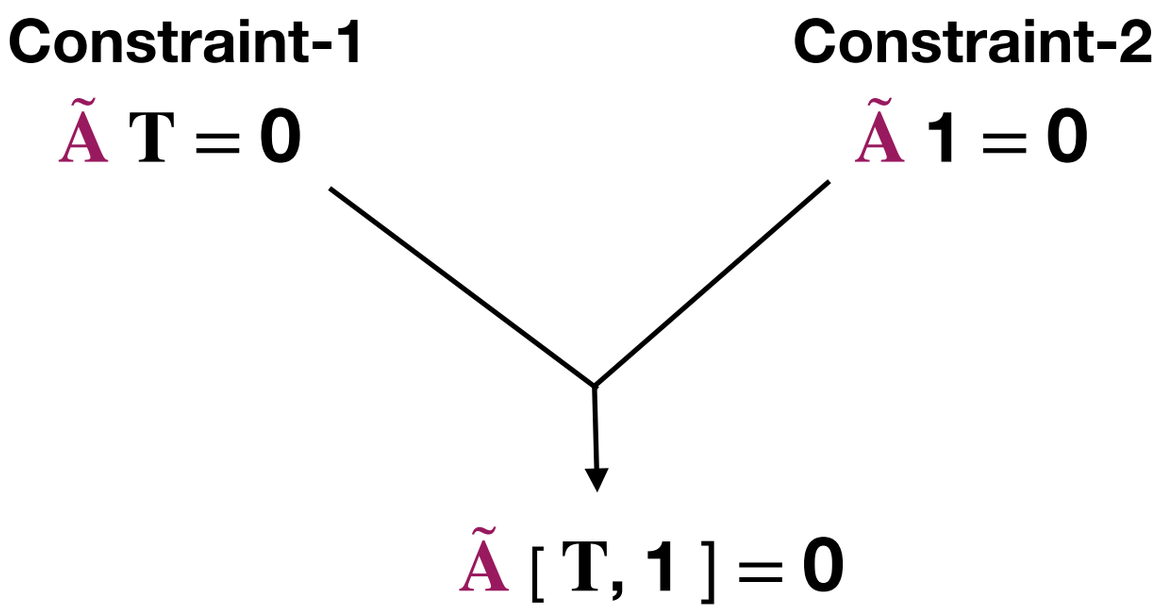

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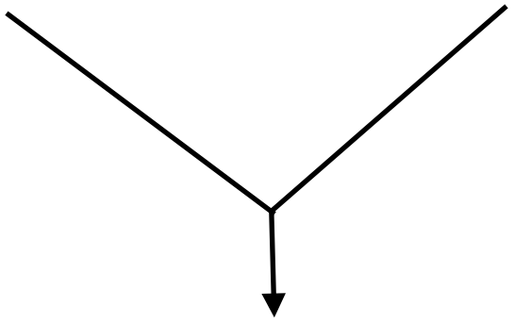

$$\tilde{\mathbf{A}}\ [\ \mathbf{T}, \mathbf{1}\ ] = \mathbf{0}$$

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($\tilde{\mathbf{a}}$ is a row of $\tilde{\mathbf{A}}$)

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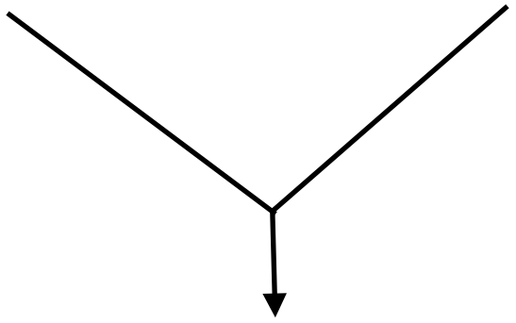

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$$\Longrightarrow \tilde{\mathbf{a}}\ [\ \mathbf{T}, \mathbf{1}\ ] = \mathbf{0} \qquad (\tilde{\mathbf{a}} \text{ is a row of } \tilde{\mathbf{A}})$$

$\tilde{\mathbf{a}}$ lies in the left null space of $[\ \mathbf{T}, \mathbf{1}\ ]$, i.e., LN($[\ \mathbf{T}, \mathbf{1}\ ]$). (for $\tilde{\mathbf{a}} \neq \mathbf{0}$)

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$\leq d_v + 1$

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$\leq d_v + 1$

$\geq d_s - d_v - 1$

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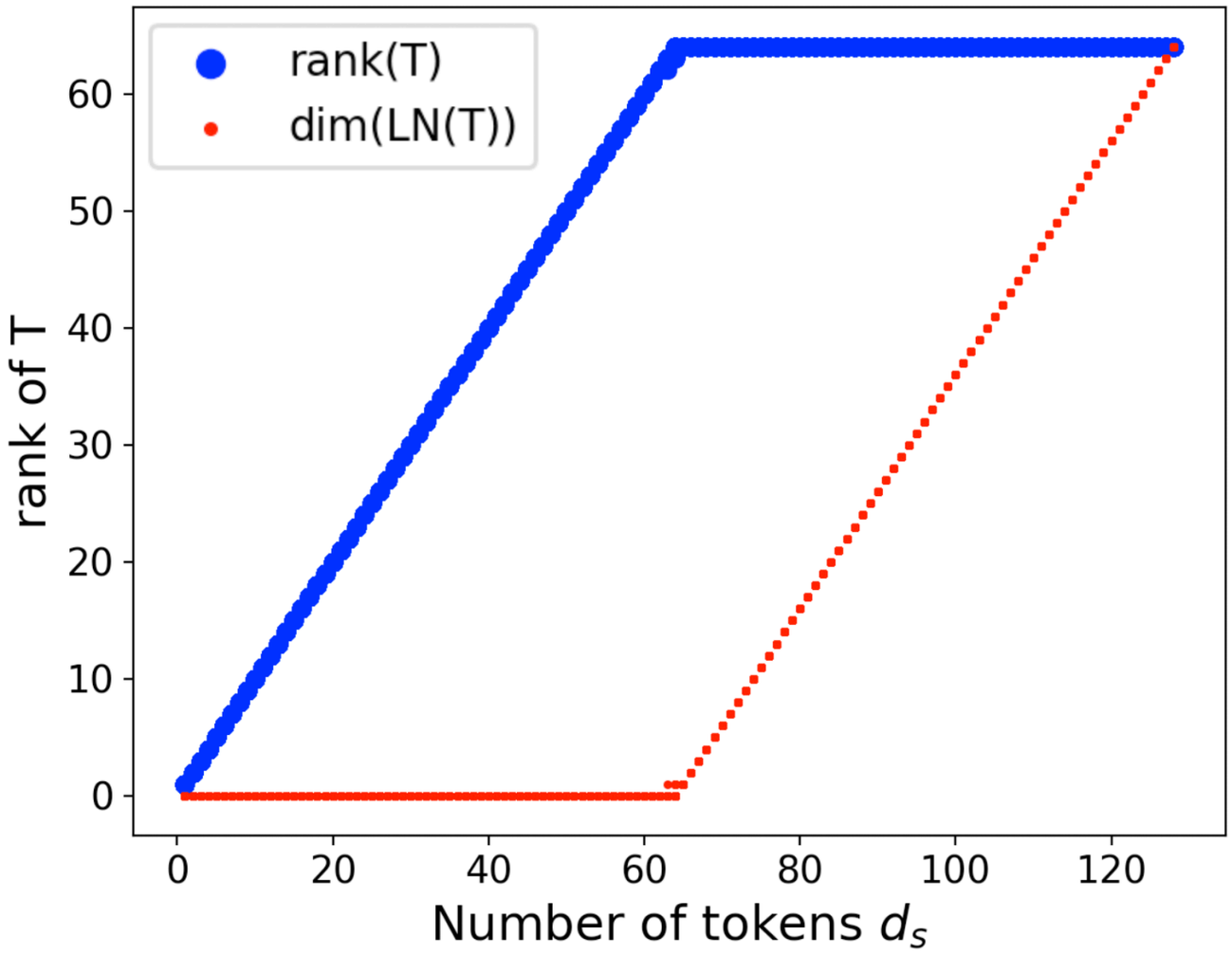
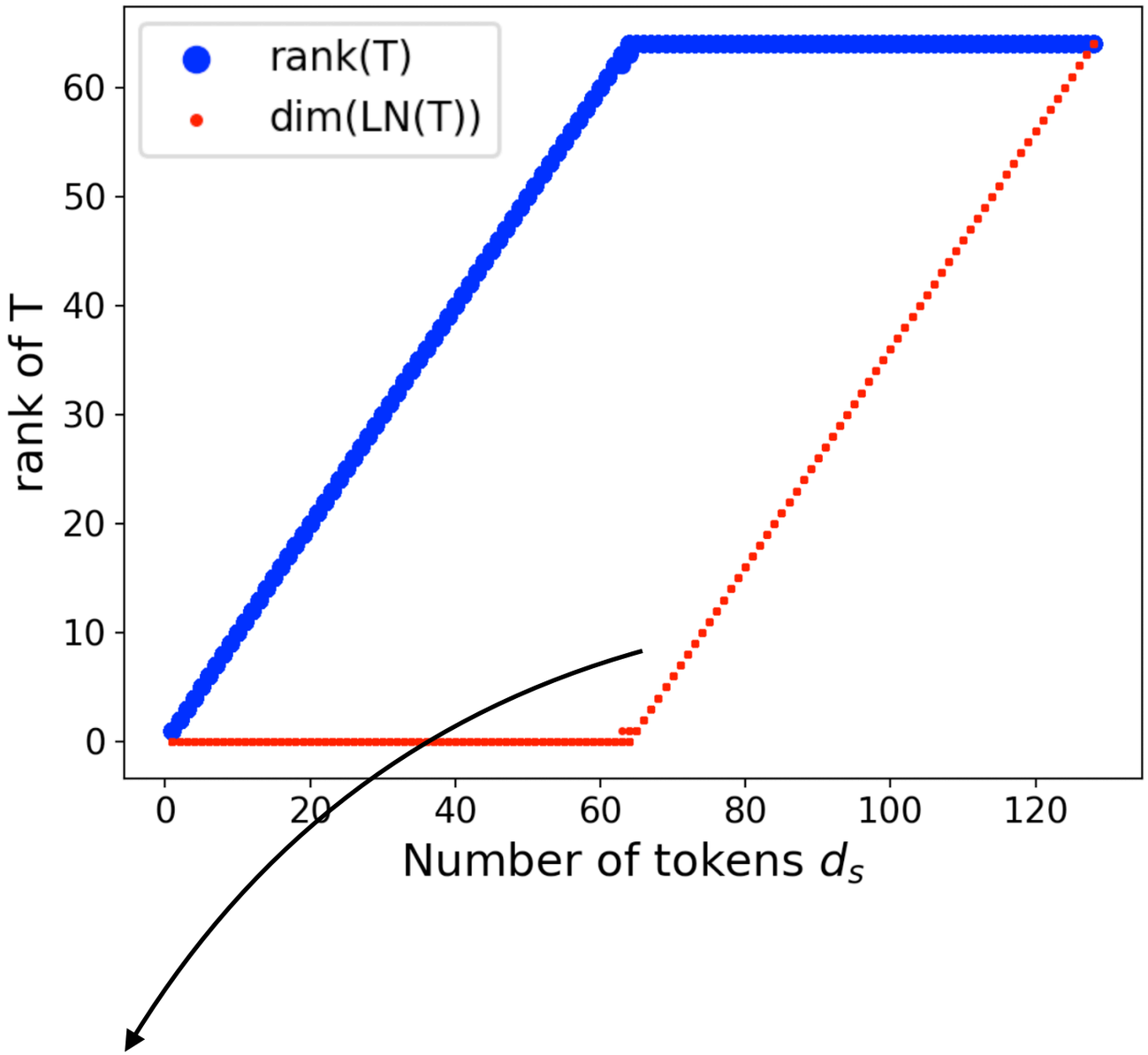


Numerical rank of $\mathbf{T}$ and dim (LN($\mathbf{T}$)) on IMDB dataset.

Uniqueness of A



$\tilde{\mathbf{a}}$ is obtainable satisfying all the Constraints 1,2, and 3 $\Longrightarrow$ $\tilde{\mathbf{A}}$ is not unique

-On identifiability in transformers [Brunner et al., 2019]

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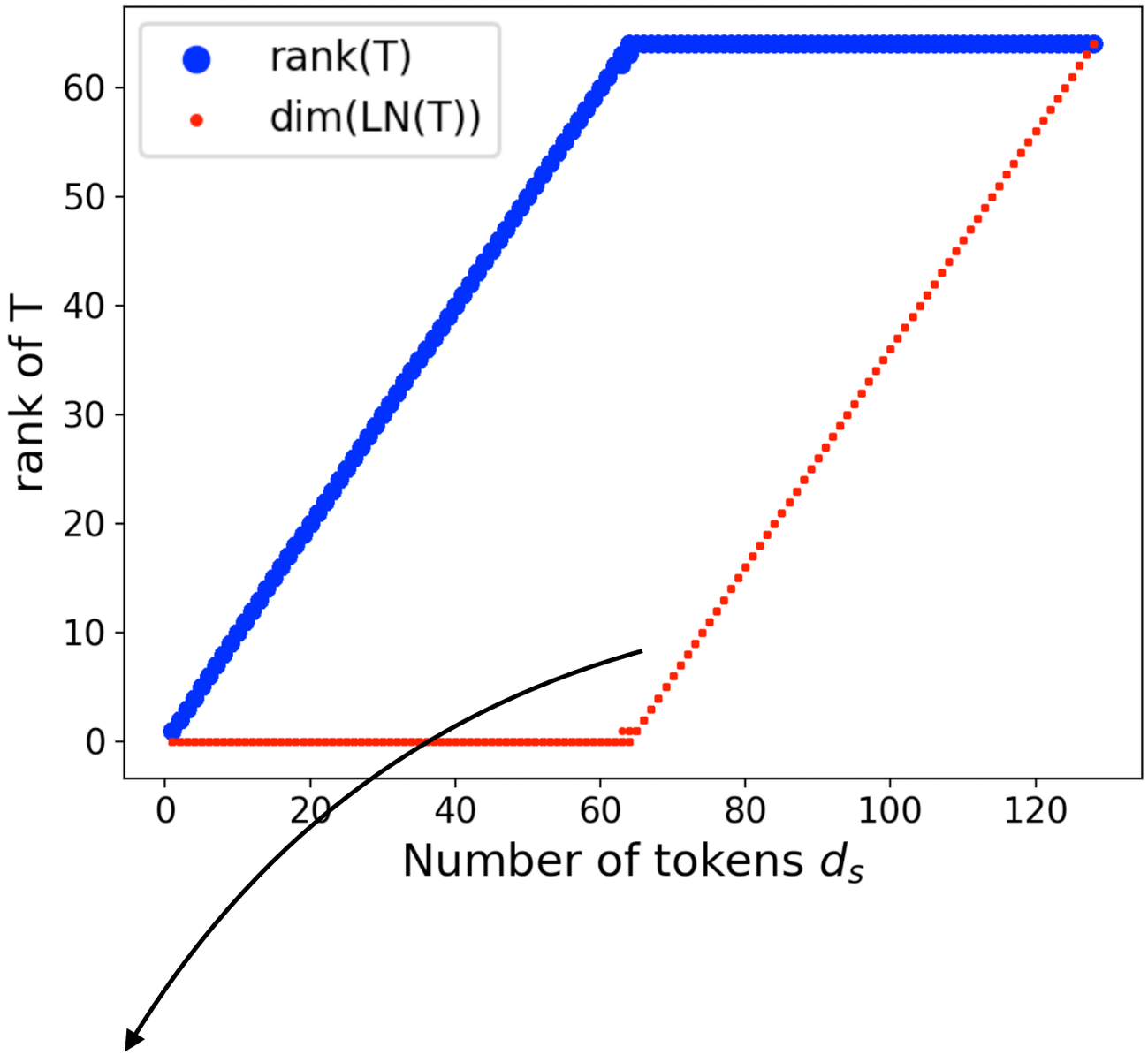

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We show that this may not be a valid claim!

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(Role of key vector size)

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Constraints 1, 2 and 3

↓ for $d_s > d_v + 1$

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Can I obtain this attention matrix from the first phase?

$$\text{softmax}\left(\frac{\mathbf{Q}\,\mathbf{K}^T}{\sqrt{d_q}}\right)$$

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↑

softmax (log($\mathbf{A} + \tilde{\mathbf{A}}$) + $\mathbf{C}$)

C: value that is constant across a row.

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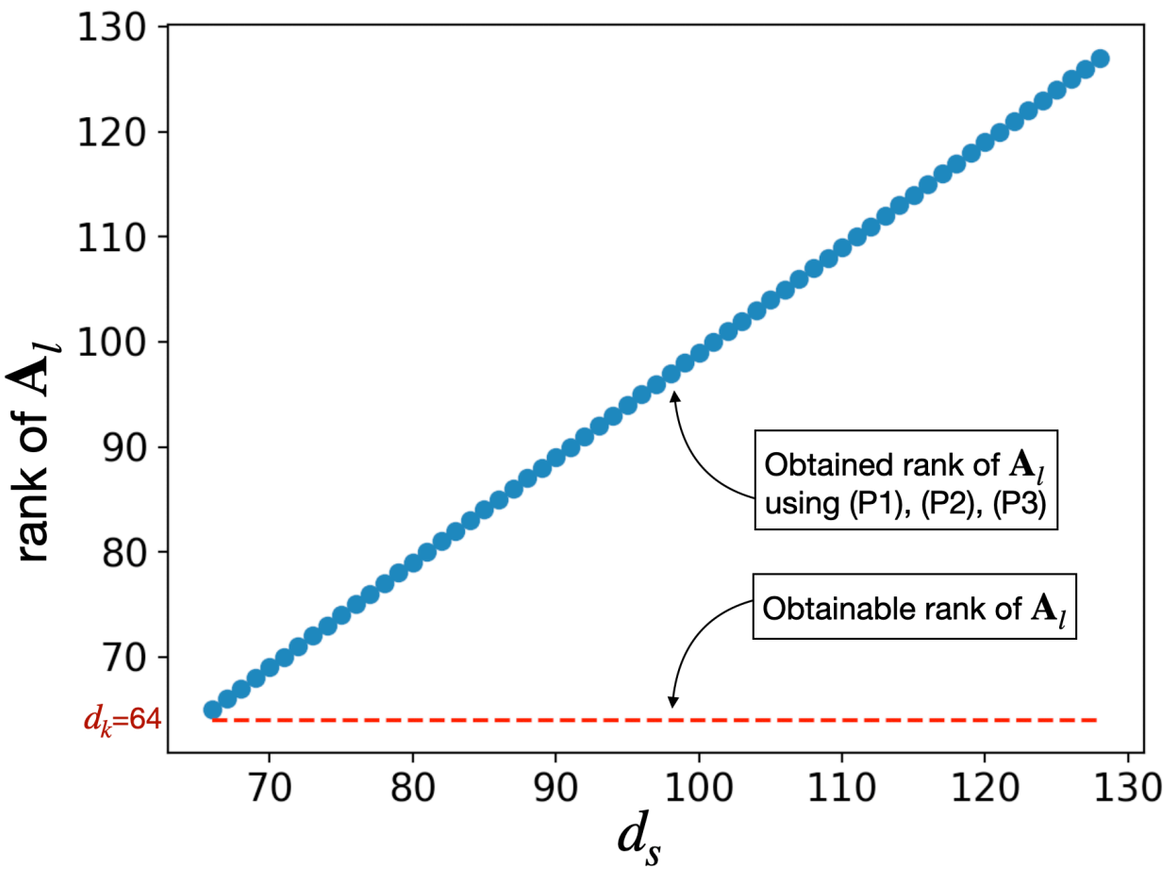

obtainable rank $(\mathbf{A}_l) \leq \min(\, d_s\,,\, d_k)$

$\leq d_k$

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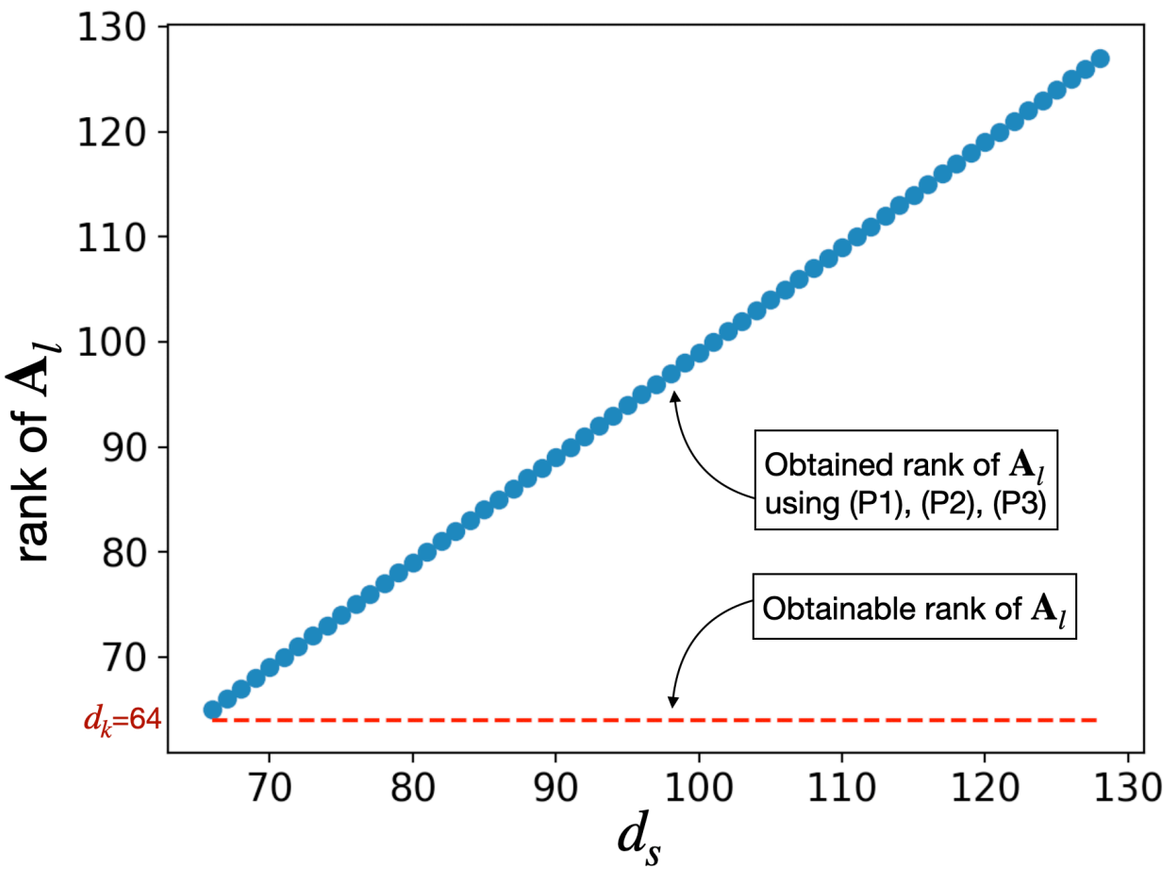

obtainable rank $(\mathbf{A}_l) \leq \min(\, d_s\,,\, d_k)$

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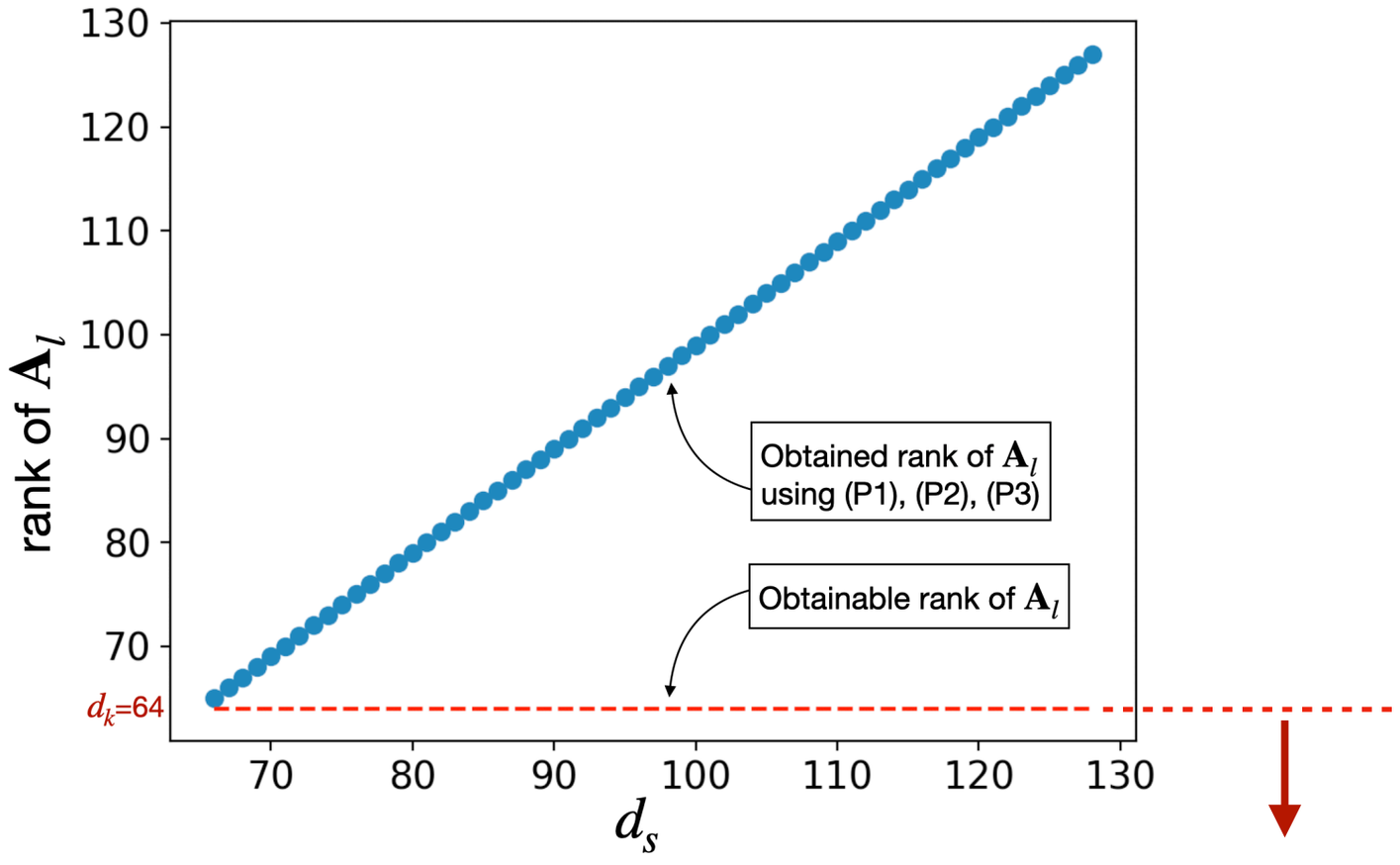
Hence, solutions satisfying constraints 1,2, and 3 may not be valid claims for A's non-uniqueness!

More identifiable

(Solution1: decrease $\mathbf{d_k}$)



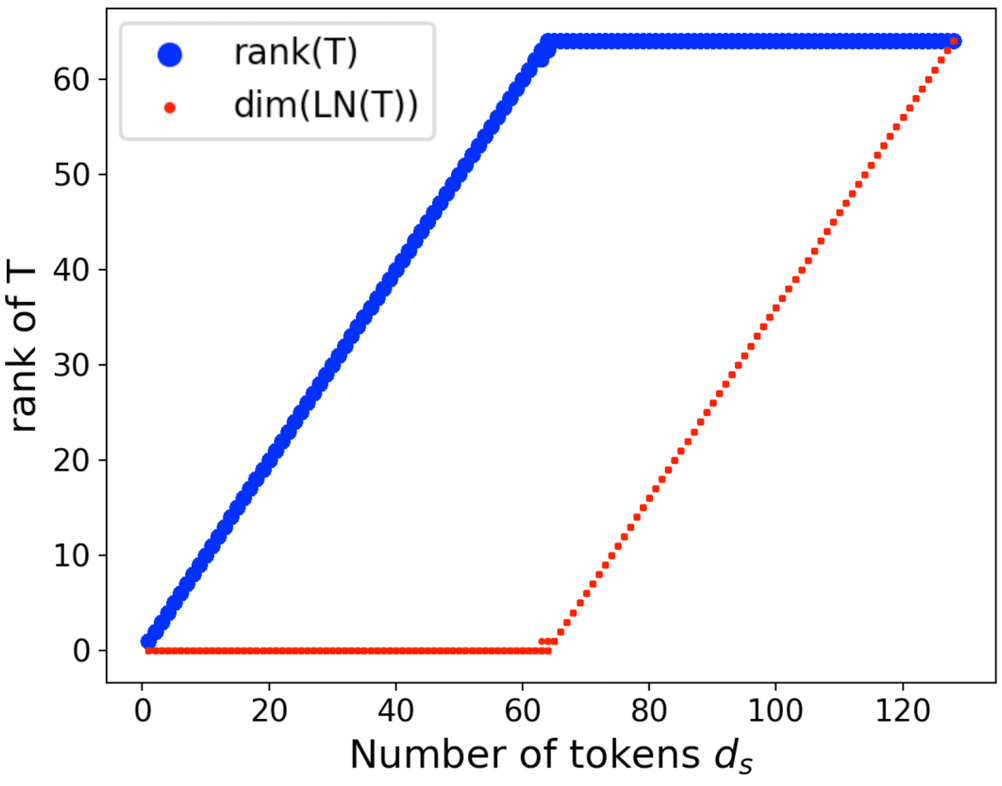
Push d_k to lower values to reduce the number of alternate attention weights ($\mathbf{A} + \tilde{\mathbf{A}}$)

More identifiable

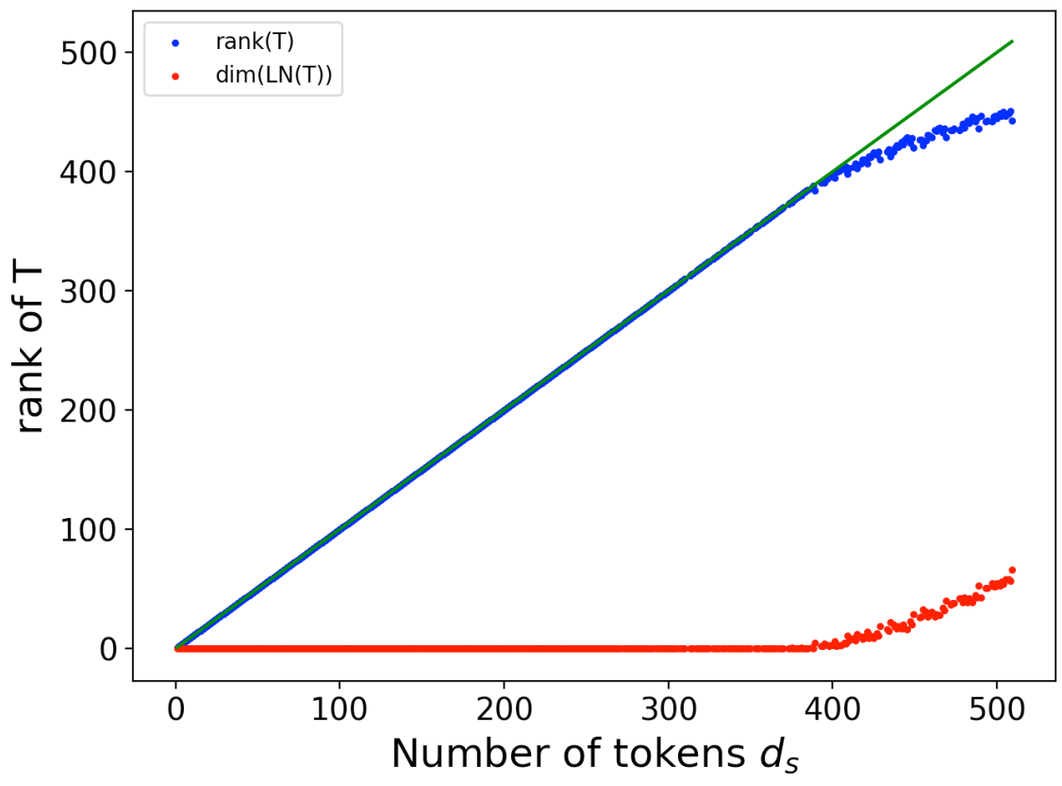
(Solution2: increase $\mathbf{d_v}$)

As $\tilde{\mathbf{A}}$ belongs to LN([$\mathbf{T}$, $\mathbf{1}$])

dim LN([$\mathbf{T}$, $\mathbf{1}$]) = d_s – rank([$\mathbf{T}$, $\mathbf{1}$])



$d_v = 64$



$d_v = 512$

Increase d_v and substitute concatenation of attention heads with addition.

Text-classification

Dataset	Version	Size of key vector (d_k)								
		1	**2**	**4**	**8**	**16**	**32**	**64**	**128**	**256**
IMDB	*Con*	0.884	0.888	0.886	0.888	0.846	0.824	0.803	0.788	0.755
	Add	0.888	0.885	0.887	0.884	0.886	0.882	0.877	0.832	0.825
TREC	*Con*	0.836	0.836	0.840	0.822	0.823	0.764	0.786	0.706	0.737
	Add	0.841	0.842	0.835	0.842	0.841	0.836	0.809	0.809	0.771
SST	*Con*	0.643	0.625	0.627	0.609	0.603	0.582	0.574	0.573	0.554
	Add	0.599	0.618	0.628	0.633	0.628	0.629	0.592	0.581	0.586
SNLI	*Con*	0.675	0.674	0.673	0.672	0.662	0.659	0.659	0.655	0.648
	Add	0.683	0.677	0.674	0.676	0.673	0.669	0.663	0.664	0.655
Yelp	*Con*	0.913	0.911	0.907	0.898	0.879	0.862	0.857	0.849	0.837
	Add	0.914	0.915	0.916	0.914	0.915	0.916	0.910	0.909	0.891
DBPedia	*Con*	0.979	0.977	0.977	0.971	0.966	0.961	0.957	0.951	0.949
	Add	0.979	0.978	0.979	0.977	0.978	0.973	0.970	0.969	0.964
Sogou	*Con*	0.915	0.907	0.898	0.900	0.893	0.888	0.868	0.858	0.838
	Add	0.915	0.908	0.906	0.904	0.913	0.914	0.910	0.906	0.899
AG News	*Con*	0.906	0.903	0.904	0.904	0.886	0.877	0.870	0.870	0.869
	Add	0.902	0.908	0.907	0.906	0.897	0.899	0.901	0.897	0.893
Yahoo	*Con*	0.695	0.690	0.684	0.664	0.644	0.627	0.616	0.597	0.574
	Add	0.697	0.695	0.696	0.693	0.693	0.694	0.688	0.649	0.683
Amazon	*Con*	0.924	0.925	0.923	0.922	0.900	0.892	0.887	0.882	0.873
	Add	0.925	0.923	0.925	0.924	0.924	0.920	0.907	0.896	0.889

The test accuracy on varied text classification datasets spread over ten datasets.

Conclusion

- We analysed attention weights in multi-head attention for their uniqueness.
- We claimed that the existing attention identifiability analysis is not complete.
- We provided a more concrete analysis of attention weights identifiability.

- We provide solutions to make attention weights more identifiable.
- The text classification performance does not vary significantly.

Thank you!

PAPER: https://arxiv.org/pdf/2106.01269.pdf
CODE: https://github.com/declare-lab/identifiable-transformers