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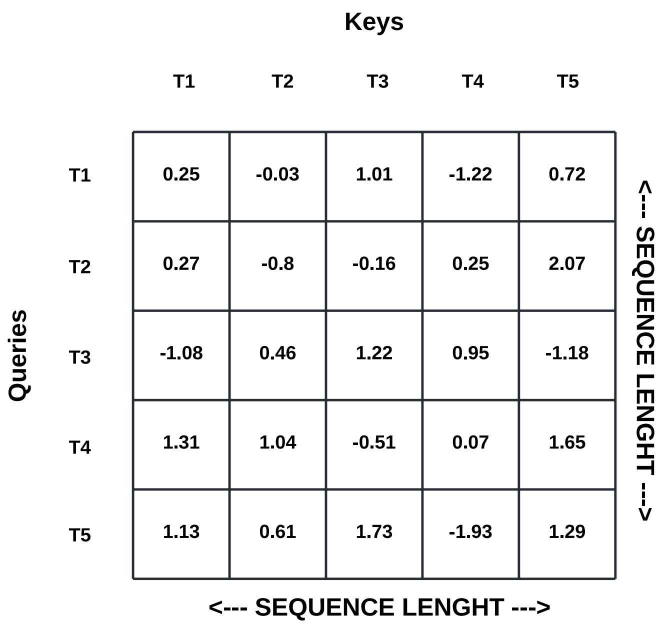
Future Attention

> NB: LaTeX here is optimized for Github's Markdown, so please view it on Github. Also, Safari does not render Github's LaTeX and some SVG files well, so Chrome is advised.

Decoder-only transformer models apply a causal mask in attention operations to enable parallel training with teacher forcing. However, the causally masked part of the attention matrix contains good signals on the affinities between present and future tokens. This project investigates how the masked part can be leveraged to improve model performance while still respecting temporal causality.

Motivations

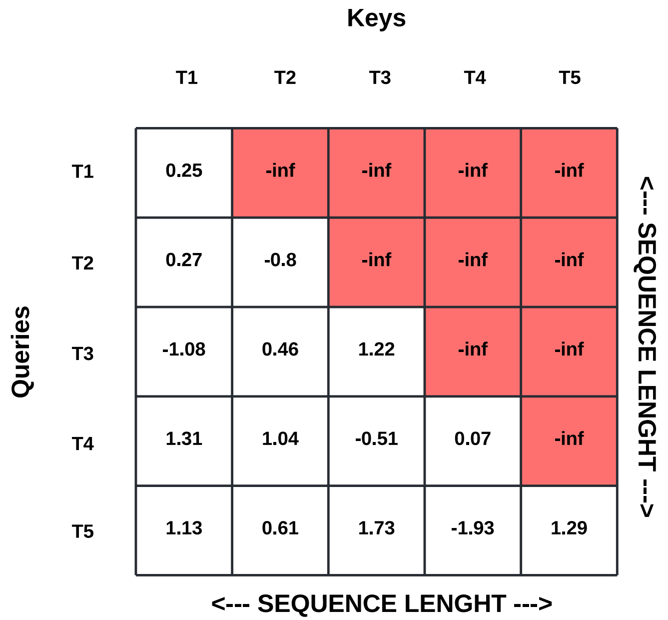
In the canonical decoder-only transformer, the attention operation computes an attention matrix A for each head, like the figure below.



Because transformer models are trained in a parallel way, a causal mask M must be applied to the attention matrix A to prevent the model from peeking at future tokens and thus from cheating. Stated more formally,

$$A_{causal}[i,j] = \begin{cases} A[i,j] & \text{if } M[i,j] = 1 \\ -\infty & \text{if } M[i,j] = 0 \end{cases}$$

The result of masking is illustrated in the figure below (the masked positions are depicted with red squares).



Afterwards, the following concludes the attention mechanism

$$out_{causal} = softmax(A_{causal}) \cdot V$$

Note: although other subsequent operations on out_{causal} usually follow (e.g. dropout, residual projection, etc.), those are not of concern here.

Before proceeding, let's identify two subsets of the original A

$$A_{unmasked}[i,j] = A[i,j] \text{ where } (i,j) \in \{(i,j) \mid M[i,j] = 1\}$$
$$A_{masked}[i,j] = A[i,j] \text{ where } (i,j) \in \{(i,j) \mid M[i,j] = 0\}$$

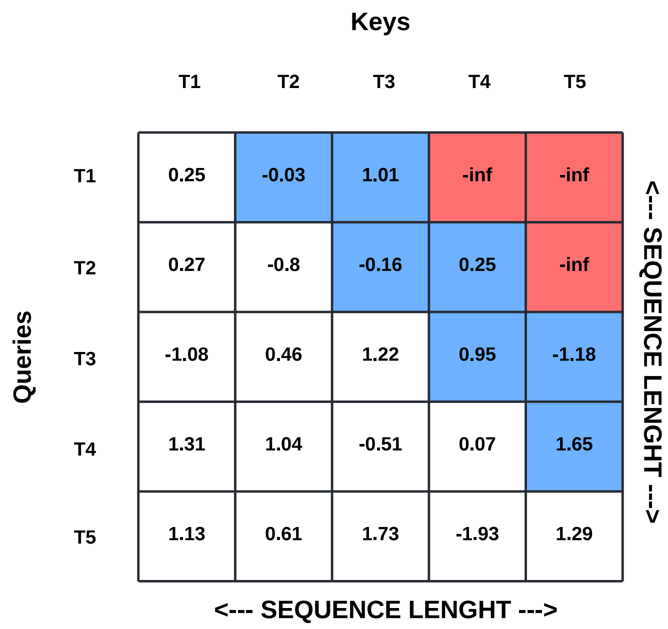
Now, the masked part A_{masked} contains good signals on the affinities between present and future tokens. If no mask M were applied, subsequent operations would transform these affinities into out_{masked}, like so

$$
\begin{aligned}
&Softmax\_A = softmax(A) \\
&Softmax\_A_{masked} = Softmax\_A[A_{masked}.indices] \\
&out_{masked} = Softmax\_A_{masked} \cdot V
\end{aligned}
$$

Presumably, the model performance would improve if it could make use of out_{masked} (i.e. add it to out_{causal}). Since the true out_{masked} can't be used because of masking, the model can instead predict out_{masked}, thus indirectly predicting A_{masked} as well. From the out_{masked} predictions, a new **future attention loss** can be formulated, with the true out^*_{masked} (which can be easily derived) as ground truth. Furthermore, instead of predicting the full out_{masked}, the model can predict part of it, which is equivalent to predicting a subset of A_{masked}. Therefore, rather than predicting out_{masked} and A_{masked}, the predictive targets become their subsets out_{future} and A_{future}, respectively. Then, let $future\_dim$ be the scalar hyperparameter that defines how many masked values in A_{masked} to predict, per token. Stated formally,

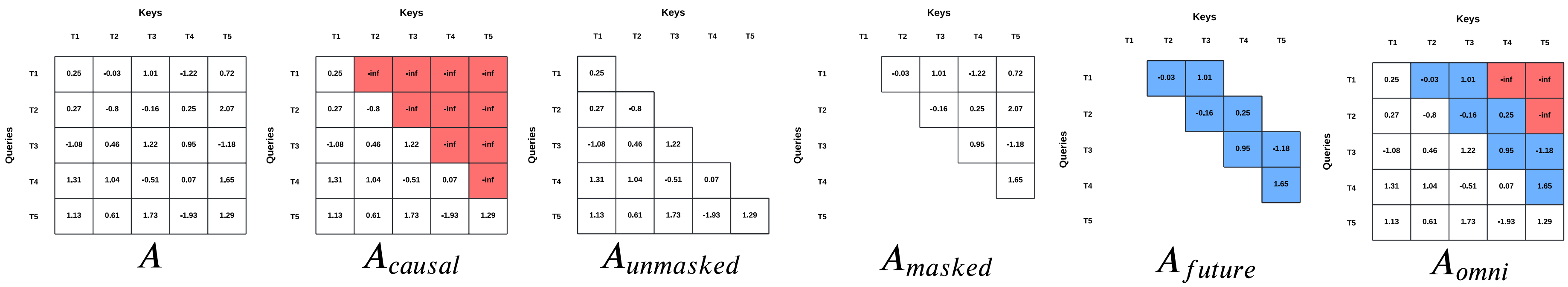
$$
\begin{aligned}
&A_{future}[i,j] = A_{masked}[i,j] \text{ where } (i,j) \in \{(i,j) \mid i < j \leq min(i + future\_dim, context\_size)\} \\
&A_{omni} = A_{future} \cup A_{unmasked} \\
\\
&Softmax\_A_{omni} = softmax(A_{omni}) \\
&Softmax\_A_{future} = Softmax\_A_{omni}[A_{future}.indices] \\
&out_{future} = Softmax\_A_{future} \cdot V
\end{aligned}
$$

In the figure below, for instance, the model tries to predict the affinity of each present token to the next two future tokens (the blue squares) while the rest is masked away (the red squares). Here, $future\_dim = 2$.



Note: $future\_dim$ only represents the max value. In fact, in the figure above, T_4 can only predict $q_4 k_5$.

Here's a visual guide for all the different attention matrices defined thus far.



(The reason for the explicit definition of all these different attention matrices is the indexing-heavy nature of the implementation presented below)

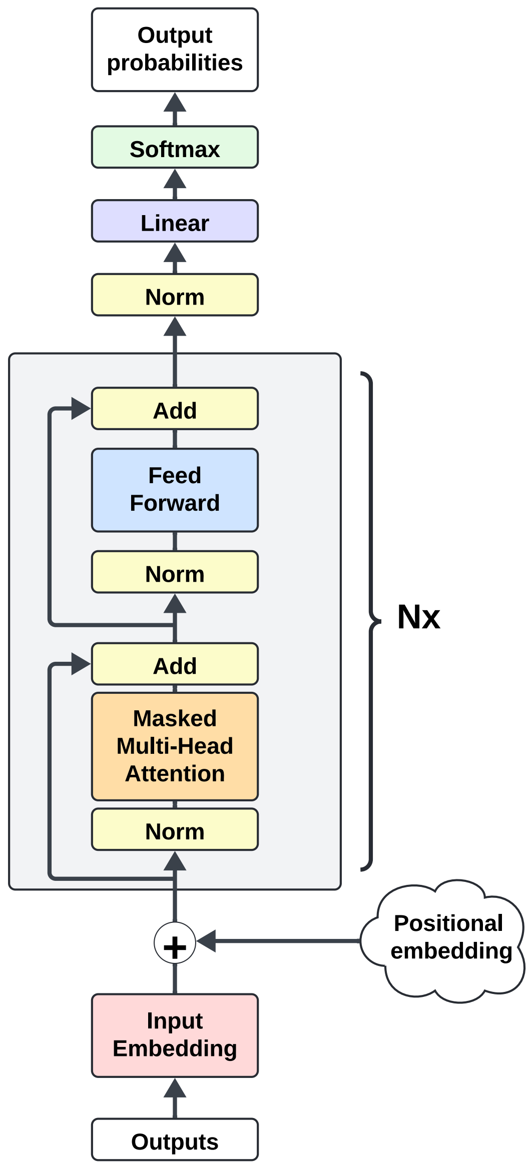
Lastly, because the softmax of the attention matrix is later matrix multiplied with V to produce the attention output out

$out = softmax(A) \cdot V$

then V also needs to be adjusted to match $Softmax\_A_{future}$'s shape.

Architecture

At the high-level, the architecture consists of a canonical decoder-only transformer with a modified multi-headed attention block that also predicts out_{future}. A new loss is created from all out_{future} predictions, in addition to the regular next token prediction loss.



Future (Multi-headed) Attention

Remember that the attention mechanism requires three operands: Q, K, and V. In predicting out_{future}, as many of these three operands as possible should be reused. In this case, Q can be reused but different K and V are needed to match A_{future} and $Softmax\_A_{future}$'s shape, respectively. Let's call these K_{future} and V_{future}. There are many ways to construct K_{future} and V_{future}, but a simple way is to have them as model parameters, not computed tensors, of shape $(n\_head \times context\_size \times head\_size)$. Parametrizing K_{future} and V_{future} is unideal because it deprives them of in-context information, but other solutions that I could think of either added too many parameters or too many operations.

Once K_{future} and V_{future} are defined, the forward pass of an attention block becomes

$A = Q \cdot K^T$	$A_{future} = Q \cdot K_{future}^T$
$A_{unmasked} = A[A_{unmasked}.indices]$	
$A_{omni} = A_{unmasked} \cup A_{future}$	
$Softmax\_A_{omni} = softmax(A_{omni})$	
$Softmax\_A_{unmasked} = Softmax\_A_{omni}[A_{unmasked}.indices]$	$Softmax\_A_{future} = Softmax\_A_{omni}[A_{future}.indices]$
$out_{unmasked} = Softmax\_A_{unmasked} \cdot V$	$out_{future} = Softmax\_A_{future} \cdot V_{future}$
$out_{omni} = out_{future} + out_{unmasked}$	

The two columns serve to highlight symmetrical operations. The order of operations goes from top to bottom

Note that $A_{unmasked}$ and A_{future} have different shapes, so merging the two requires padding operations that are hard to express in LaTeX. Also, note that $out_{unmasked} \neq out_{causal}$ because the former's softmax is on the union of $A_{unmasked}$ and A_{future}.

Then, deriving the true out^*_{future} simply becomes

$$
\begin{aligned}
&A^*_{omni} = A[A_{unmasked}.indices \cup A_{future}.indices] \\
&Softmax\_A^*_{omni} = softmax(A^*_{omni}) \\
&Softmax\_A^*_{future} = Softmax\_A^*_{omni}[A_{future}.indices] \\
&out^*_{future} = Softmax\_A^*_{future} \cdot V
\end{aligned}
$$

The future attention loss is computed between out_{future} and detached out^*_{future}, for every attention head block. Two types of loss are considered. One is mean squared error, and the other is cosine dissimilarity. Cosine dissimilarity is cosine similarity normalized such that zero represents most similarity and 1 most dissimilarity. So the future attention loss with MSE is given by

$$future\_attn\_loss = MSE(out_{future}, out^*_{future}.detached())$$

and with cosine dissimilarity is given by

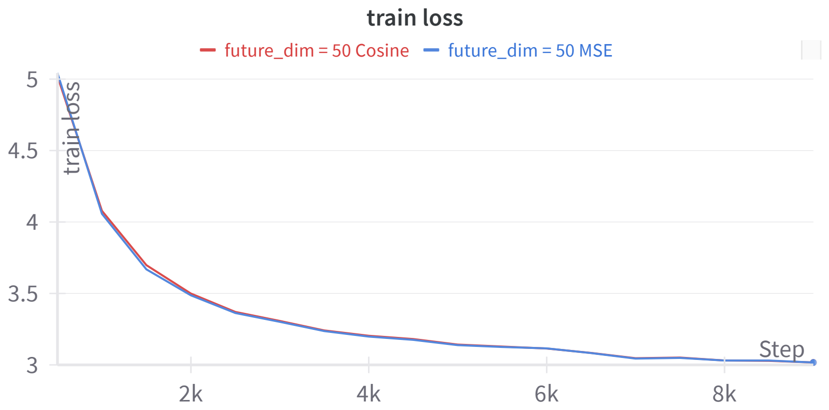
$$future\_attn\_loss = 1 - \frac{cosine\_similarity(out_{future}, out^*_{future}.detached()) + 1}{2}$$

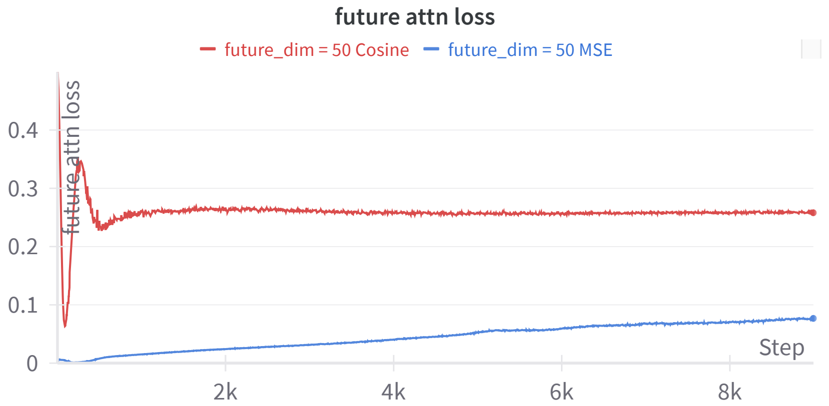
Once all $future\_attn\_loss$'s are computed, it gets aggregated with a mean and added to the model loss.

Results

> All training runs below were done on a [wikipedia dataset](#) for 9k steps on a single A100 GPU, unless otherwise stated.
>
> Implementation of decoder-only transformer model (baseline) can be found in the `baseline_transformer` directory in this repo

The MSE future attention loss outperformed cosine dissimilarity in validation loss and matched it in train loss. Both had $future\_dim = 50$.

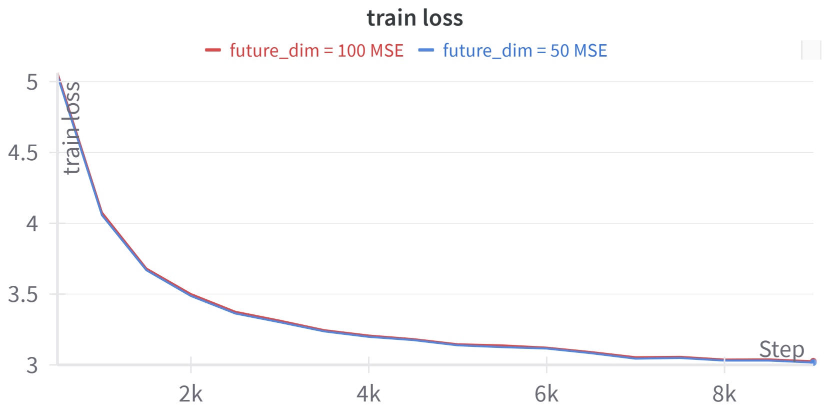


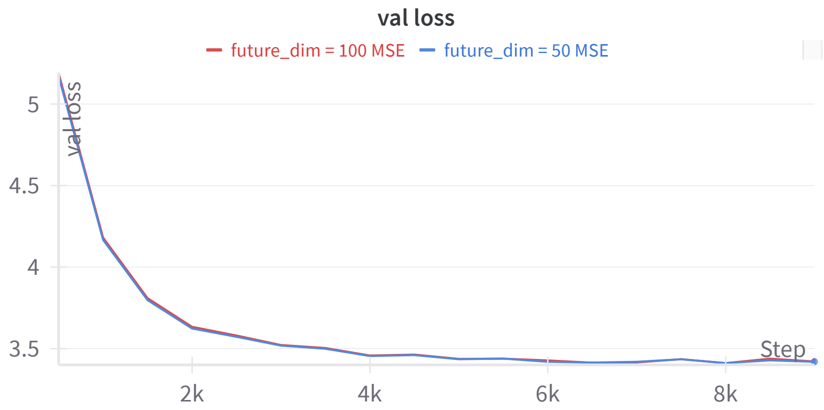


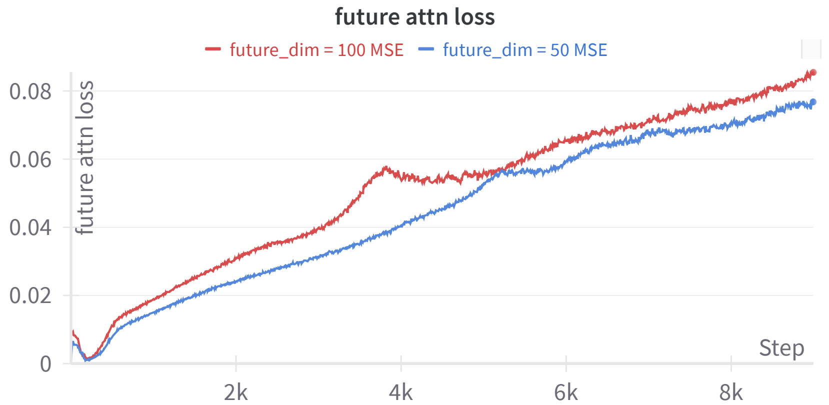
Safari may not render the charts above. Chrome is advised.

	Train loss	Val loss	Future attention loss
future_dim = 50 Cosine [(config)]()	3.017	3.423	0.2589
future_dim = 50 MSE [(config)]()	3.017	**3.419**	0.07681

With MSE future attention loss, the performances of $future\_dim = 50$ and $future\_dim = 100$ were compared. Intuitively, larger $future\_dim$ should result in better performance, but $future\_dim = 100$ underperformed across the board.



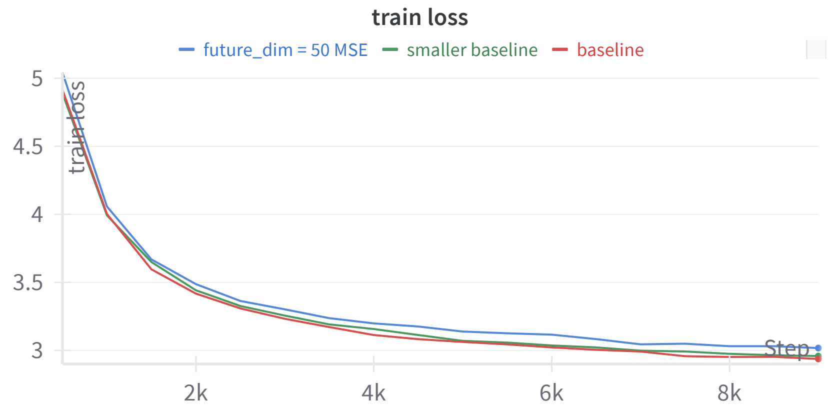


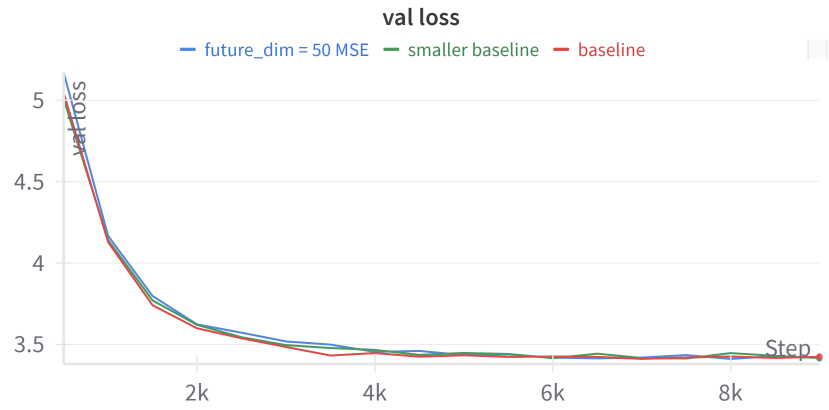


Safari may not render the charts above. Chrome is advised.

	Train loss	Val loss	Future attention loss
future_dim = 50 MSE [(config)]()	**3.017**	**3.419**	0.07681
future_dim = 100 MSE [(config)]()	3.025	3.421	0.08633

Finally, the new model was compared with a canonical decoder-only transformer (baseline). There were two versions of the baseline: "baseline" and "smaller baseline". "baseline" had more parameters than the new model. "smaller baseline" had fewer parameters. The new model outperformed "baseline" in validation loss but underperformed "smaller baseline".





Safari may not render the charts above. Chrome is advised.

	Train loss	Val loss	Size (params)
future_dim = 50 MSE [(config)]()	3.017	3.419	15,817,248
baseline [(config)]()	**2.937**	3.424	16,036,800
smaller baseline [(config)]()	2.958	**3.416**	15,441,192

Next steps

These are some improvements to look forward to:

- let K_{future} and V_{future} be computed values (just like Q, K, and V). Should also do this in a parameter count efficient way (ideally reusing or closely deriving from K and V)
- instead of MSE and cosine dissimilarity, consider other loss types

- try bigger models, at least GPT-2 size
- run training for longer to observe long-term behavior
- evaluate on different datasets
- evaluate on non-language tasks

Conclusions

This project was inspired by an accident where I forgot to apply the causal mask to a model. My overjoy for the spectacular model performance quickly evaporated upon the discovery of the bug. Yet, I wondered if there were a way to respect temporal causality while still taking advantage of the full attention matrix. Unfortunately, the results of this project do not corroborate this idea.

I believe the results were poor for two reasons: 1) bad K_{future} and V_{future} construction, and 2) bad future attention loss formulation. For 1), remember that the attention mechanism only makes sense when using in-context information, which is why Q, K, and V are all computed values. However, the parametrization of K_{future} and V_{future} deprives them of in-context information. Therefore, K_{future} and V_{future} probably have to compress all possible K and V values into their weights and/or heavily rely on Q. Furthermore, perhaps it may not even make sense to predict the masked attention with another attention operation.

For 2), the future attention loss uses out^*_{future} as ground truth, which is basically a hidden state and thus very transient. Moreover, since different model layers specialize in different things, the out^*_{future} of each attention block is probably very different from the others, further aggravated by out^*_{future}'s transience. All of this, coupled with the future attention loss being computed for all L layers, means that, instead of a single "future attention" objective function, there are essentially L orthogonally different objective functions. Indeed, all future attention loss charts either show increasing loss or some equilibrium point, and none showed convergence towards zero loss.

The first reason is amenable to change, but the second one is probably inevitable. Alas, the principal limitation is my personal compute budget, so this project cannot avail itself of further analysis and experimentation.

Citation

If you use this codebase, or otherwise found my work valuable, please cite:

```
@misc{yan2024future-attention,
  title={Future Attention},
  author={Yan, Yifei},
  year={2024},
  url={https://github.com/yiphei/yif-AI/tree/main/future_attention}
}
```

Appendix

Run configs

"future_dim = 50 Cosine"

```
batch_size: 50
beta1: 0.9
beta2: 0.95
decay_lr: true
est_interval: 500
est_steps: 200
gradient_accumulation_steps: 16
lr: 0.0009
lr_decay_iters: 700000
min_lr: 9.0e-05
model_config:
  context_size: 200
  detach_future_ground_truth: true
```

```
    dropout_rate: 0
    end_layer: 28
    future_attn_loss_coeff: 1
    future_attn_loss_type: "COSINE"
    future_dim: 50
    n_embed: 144
    n_head: 9
    n_layer: 28
    start_layer: 1
    use_bias: false
    use_future_attn_loss: true
  train_steps: 9000
  warmup_iters: 300
  weight_decay: 0.1
```

"future_dim = 50 MSE"

```
  batch_size: 50
  beta1: 0.9
  beta2: 0.95
  decay_lr: true
  est_interval: 500
  est_steps: 200
  gradient_accumulation_steps: 16
  lr: 0.0009
  lr_decay_iters: 700000
  min_lr: 9.0e-05
  model_config:
    context_size: 200
    detach_future_ground_truth: true
    dropout_rate: 0
    end_layer: 28
    future_attn_loss_coeff: 1
```

```
    future_attn_loss_type: "MSE"
    future_dim: 50
    n_embed: 144
    n_head: 9
    n_layer: 28
    start_layer: 1
    use_bias: false
    use_future_attn_loss: true
  train_steps: 9000
  warmup_iters: 300
  weight_decay: 0.1
```

"future_dim = 100 MSE"

```
  batch_size: 50
  beta1: 0.9
  beta2: 0.95
  decay_lr: true
  est_interval: 500
  est_steps: 200
  gradient_accumulation_steps: 16
  lr: 0.0009
  lr_decay_iters: 700000
  min_lr: 9.0e-05
  model_config:
    context_size: 200
    detach_future_ground_truth: true
    dropout_rate: 0
    end_layer: 28
    future_attn_loss_coeff: 1
    future_attn_loss_type: "MSE"
    future_dim: 100
    n_embed: 144
```

```
    n_head: 9
    n_layer: 28
    start_layer: 1
    use_bias: false
    use_future_attn_loss: true
  train_steps: 9000
  warmup_iters: 300
  weight_decay: 0.1
```

"baseline"

```
  batch_size: 50
  beta1: 0.9
  beta2: 0.95
  decay_lr: true
  est_interval: 500
  est_steps: 200
  gradient_accumulation_steps: 16
  lr: 0.0009
  lr_decay_iters: 700000
  min_lr: 9.0e-05
  model_config:
    context_size: 200
    dropout_rate: 0
    n_embed: 160
    n_head: 10
    n_layer: 26
    use_bias: false
  train_steps: 9000
  warmup_iters: 300
  weight_decay: 0.1
```

"smaller baseline"

```
batch_size: 50
beta1: 0.9
beta2: 0.95
decay_lr: true
est_interval: 500
est_steps: 200
gradient_accumulation_steps: 16
lr: 0.0009
lr_decay_iters: 700000
min_lr: 9.0e-05
model_config:
  context_size: 200
  dropout_rate: 0
  n_embed: 156
  n_head: 12
  n_layer: 26
  use_bias: false
train_steps: 9000
warmup_iters: 300
weight_decay: 0.1
```