XLNet: Generalized Autoregressive Pretraining for Language Understanding¹

June 21, 2019



 $^{^1\}it{XLNet}$: Generalized Autoregressive Pretraining for Language Understanding by Yang et al.





 $^{^2}$ That's why we also predict non-mask tokens during pretraining.

³besides obesity

1. It predicts MASK tokens independently, i.e. $p(\tilde{\mathbf{x}}|\hat{\mathbf{x}}) = \prod_{i=1}^{T} p(\tilde{x}_i|\hat{\mathbf{x}})$, where $\tilde{\mathbf{x}}, \hat{\mathbf{x}}$ are masked and unmasked subsequences of \mathbf{x} . It's a big deal, because in reality:

$$p(\mathsf{New},\mathsf{York}|\hat{\boldsymbol{x}}) = p(\mathsf{New}|\hat{\boldsymbol{x}}) \cdot p(\mathsf{York}|\mathsf{New},\hat{\boldsymbol{x}}) \neq p(\mathsf{New}|\hat{\boldsymbol{x}}) \cdot p(\mathsf{York}|\hat{\boldsymbol{x}})$$



²That's why we also predict non-mask tokens during pretraining.

³besides obesity

1. It predicts MASK tokens independently, i.e. $p(\tilde{x}|\hat{x}) = \prod_{i=1}^{T} p(\tilde{x}_i|\hat{x})$, where \tilde{x}, \hat{x} are masked and unmasked subsequences of x. It's a big deal, because in reality:

$$p(\mathsf{New},\mathsf{York}|\hat{\boldsymbol{x}}) = p(\mathsf{New}|\hat{\boldsymbol{x}}) \cdot p(\mathsf{York}|\mathsf{New},\hat{\boldsymbol{x}}) \neq p(\mathsf{New}|\hat{\boldsymbol{x}}) \cdot p(\mathsf{York}|\hat{\boldsymbol{x}})$$

2. In test time we do not have MASK tokens, which is train-test discrepancy!²



²That's why we also predict non-mask tokens during pretraining.

³besides obesity

1. It predicts MASK tokens independently, i.e. $p(\tilde{x}|\hat{x}) = \prod_{i=1}^{T} p(\tilde{x}_i|\hat{x})$, where \tilde{x}, \hat{x} are masked and unmasked subsequences of x. It's a big deal, because in reality:

$$p(\mathsf{New},\mathsf{York}|\hat{\boldsymbol{x}}) = p(\mathsf{New}|\hat{\boldsymbol{x}}) \cdot p(\mathsf{York}|\mathsf{New},\hat{\boldsymbol{x}}) \neq p(\mathsf{New}|\hat{\boldsymbol{x}}) \cdot p(\mathsf{York}|\hat{\boldsymbol{x}})$$

- 2. In test time we do not have MASK tokens, which is train-test discrepancy!²
- 3. Using large contexts is very costly $O(n^2)$.



²That's why we also predict non-mask tokens during pretraining.

³besides obesity



▶ We can train them either forward or backward⁴



- ▶ We can train them either forward or backward⁴
- ▶ ⇒ model is not trained to use the whole context



- ▶ We can train them either forward or backward⁴
- ▶ ⇒ model is not trained to use the whole context
- → it's bad, because such an information is very useful for some tasks



⁴or bidirectionally with simple concatenation, like ELMO



▶ Let \mathcal{Z}_T be a set of all possible permutations of a sequence of length T (so it has T! elements).



- ▶ Let \mathcal{Z}_T be a set of all possible permutations of a sequence of length T (so it has T! elements).
- Note that we can decompose p(x) via chain rule in an arbitrary order:

$$p(\mathbf{x}) = p(x_1, x_2, x_3)$$

$$= p(x_1)p(x_2|x_1)p(x_3|x_1, x_2)$$

$$= p(x_2)p(x_3|x_2)p(x_1|x_2, x_3)$$

$$= \dots$$



- ▶ Let \mathcal{Z}_T be a set of all possible permutations of a sequence of length T (so it has T! elements).
- Note that we can decompose p(x) via chain rule in an arbitrary order:

$$p(\mathbf{x}) = p(x_1, x_2, x_3)$$

$$= p(x_1)p(x_2|x_1)p(x_3|x_1, x_2)$$

$$= p(x_2)p(x_3|x_2)p(x_1|x_2, x_3)$$

$$= \dots$$

▶ Which order is the best for our task? Forward? Backward?



- Let \mathcal{Z}_T be a set of all possible permutations of a sequence of length T (so it has T! elements).
- Note that we can decompose p(x) via chain rule in an arbitrary order:

$$p(\mathbf{x}) = p(x_1, x_2, x_3)$$

$$= p(x_1)p(x_2|x_1)p(x_3|x_1, x_2)$$

$$= p(x_2)p(x_3|x_2)p(x_1|x_2, x_3)$$

$$= \dots$$

- ▶ Which order is the best for our task? Forward? Backward?
- All of them:

$$\mathcal{L}_{\mathsf{XLNet}}(heta) = - \underset{oldsymbol{z} \sim \mathcal{Z}_{\mathcal{T}}}{\mathbb{E}} \left[\log p_{ heta}(oldsymbol{x})
ight] = - \underset{oldsymbol{z} \sim \mathcal{Z}_{\mathcal{T}}}{\mathbb{E}} \left[\sum_{t=1}^{I} \log p_{ heta}(oldsymbol{x}_{z_t} | oldsymbol{x}_{oldsymbol{z}_{< t}})
ight]$$



- Let \mathcal{Z}_T be a set of all possible permutations of a sequence of length T (so it has T! elements).
- Note that we can decompose p(x) via chain rule in an arbitrary order:

$$p(\mathbf{x}) = p(x_1, x_2, x_3)$$

$$= p(x_1)p(x_2|x_1)p(x_3|x_1, x_2)$$

$$= p(x_2)p(x_3|x_2)p(x_1|x_2, x_3)$$

$$= \dots$$

- ▶ Which order is the best for our task? Forward? Backward?
- All of them:

$$\mathcal{L}_{\mathsf{XLNet}}(heta) = - \underset{oldsymbol{z} \sim \mathcal{Z}_{\mathcal{T}}}{\mathbb{E}}[\log p_{ heta}(oldsymbol{x})] = - \underset{oldsymbol{z} \sim \mathcal{Z}_{\mathcal{T}}}{\mathbb{E}}\left[\sum_{t=1}^{T} \log p_{ heta}(oldsymbol{x}_{oldsymbol{z}_{t}} | oldsymbol{x}_{oldsymbol{z}_{c}})
ight]$$

▶ Is this an upper bound for a true loss? Yes:

$$\mathbb{E}_{\mathbf{z}}[\log p(\mathbf{x}|\mathbf{z})] \leq \log \mathbb{E}_{\mathbf{z}}[p(\mathbf{x}|\mathbf{z})] = \log p(\mathbf{x})$$





▶ It's straight-forward how to decode the sequence in the required order *z*: just use proper masks



▶ It's straight-forward how to decode the sequence in the required order z: just use proper masks

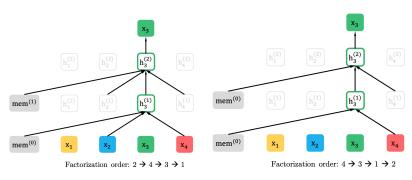


Figure: Example of prediction token x_3 for different permutation orders z.





▶ But we cannot predict "next" token like we do in language models!



- ▶ But we cannot predict "next" token like we do in language models!
- ▶ Because we have many possible permutations, the same hidden state will be used to predict different tokens:

$$\begin{aligned} \mathbf{z}^{(1)} &= (3,4,2,1,5) \\ \mathbf{z}^{(2)} &= (3,4,2,5,1) \end{aligned} \Longrightarrow \begin{cases} p(x_1 = s | x_3, x_4, x_2) = \frac{\exp(e(x)^{\top} h_{\theta}(\mathbf{x}_2 < t))}{\sum_{x'} \exp(e(x')^{\top} h_{\theta}(\mathbf{x}_2 < t))} \\ p(x_5 = s | x_3, x_4, x_2) = \frac{\exp(e(x)^{\top} h_{\theta}(\mathbf{x}_2 < t))}{\sum_{x'} \exp(e(x')^{\top} h_{\theta}(\mathbf{x}_2 < t))} \end{cases}$$



- ▶ But we cannot predict "next" token like we do in language models!
- ▶ Because we have many possible permutations, the same hidden state will be used to predict different tokens:

Solution?



- ▶ But we cannot predict "next" token like we do in language models!
- ▶ Because we have many possible permutations, the same hidden state will be used to predict different tokens:

▶ Solution? Predict token from additional [MASK] embedding.



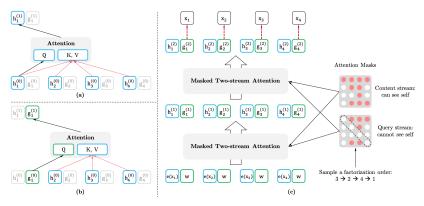


Figure: Two-stream self-attention (copy pasted for intensive hand waving).





▶ For each sentence in a batch take a random permutation $z \in \mathcal{Z}_T$ for decoding.



- ▶ For each sentence in a batch take a random permutation $z \in \mathcal{Z}_T$ for decoding.
- ▶ Initialize [MASK] tokens with trained embeddings.



- ▶ For each sentence in a batch take a random permutation $z \in \mathcal{Z}_T$ for decoding.
- ▶ Initialize [MASK] tokens with trained embeddings.
- Use forward/backward pass for each half of the batch (explained later).



- ▶ For each sentence in a batch take a random permutation $z \in \mathcal{Z}_T$ for decoding.
- ▶ Initialize [MASK] tokens with trained embeddings.
- Use forward/backward pass for each half of the batch (explained later).
- ▶ Mask around 15% of tokens (because otherwise it will be hard to train).



- ▶ For each sentence in a batch take a random permutation $z \in \mathcal{Z}_T$ for decoding.
- ▶ Initialize [MASK] tokens with trained embeddings.
- Use forward/backward pass for each half of the batch (explained later).
- ▶ Mask around 15% of tokens (because otherwise it will be hard to train).
- ▶ We use [A, SEP, B, SEP, CLS] like in BERT.



- ▶ For each sentence in a batch take a random permutation $z \in \mathcal{Z}_T$ for decoding.
- ▶ Initialize [MASK] tokens with trained embeddings.
- Use forward/backward pass for each half of the batch (explained later).
- ▶ Mask around 15% of tokens (because otherwise it will be hard to train).
- ▶ We use [A, SEP, B, SEP, CLS] like in BERT.
- ▶ We use relative segment encoding: $a_{ij}^{\text{final}} = a_{ij} + (\boldsymbol{q}_i + \boldsymbol{b})^{\top} \boldsymbol{s}_{ij}$, where \boldsymbol{q}_i is our query, \boldsymbol{b} is a learned head-specific vector, $\boldsymbol{s}_{ij} = \boldsymbol{s}_{-}$ or \boldsymbol{s}_{+} if i is in the same context as j or not.





- ► Key idea: make information about position be dependent only on relative positions between objects, regardless where they are placed in the sequence
- ▶ Why do we need this?



- Key idea: make information about position be dependent only on relative positions between objects, regardless where they are placed in the sequence
- ▶ Why do we need this? To attend on memory without much trouble (memory usually has the same positional embeddings).



- Key idea: make information about position be dependent only on relative positions between objects, regardless where they are placed in the sequence
- ▶ Why do we need this? To attend on memory without much trouble (memory usually has the same positional embeddings).
- ▶ Imagine we have hidden states e_i , e_j . We add positional embeddings to them: $h_i = e_i + p_i$ and $h_j = e_j + p_j$



(from Transformer-XL)

- ▶ Key idea: make information about position be dependent only on relative positions between objects, regardless where they are placed in the sequence
- ▶ Why do we need this? To attend on memory without much trouble (memory usually has the same positional embeddings).
- ▶ Imagine we have hidden states e_i , e_j . We add positional embeddings to them: $h_i = e_i + p_i$ and $h_j = e_j + p_j$

Then normal attention of h_i on h_j is computed as

$$Attn(\mathbf{h}_i, \mathbf{h}_j) = \langle W_q \mathbf{h}_i, W_k \mathbf{h}_j \rangle = \langle W_q(\mathbf{e}_i + \mathbf{p}_i), W_k(\mathbf{e}_j + \mathbf{p}_j) \rangle$$

$$= \mathbf{e}_i^\top W_q^\top W_k \mathbf{e}_j + \mathbf{e}_i^\top W_q^\top W_k \mathbf{p}_j + \mathbf{p}_i^\top W_q^\top W_k \mathbf{e}_j + \mathbf{p}_i^\top W_q^\top W_k \mathbf{p}_j$$

Relative positional encoding just changes attention mechanism to:

$$\mathsf{Attn}^{\mathsf{rel}}(\boldsymbol{h}_i, \boldsymbol{h}_j) = \boldsymbol{e}_i^\top W_q^\top W_k^{\boldsymbol{e}} \boldsymbol{e}_j + \boldsymbol{e}_i^\top W_q^\top W_k^{\boldsymbol{r}} \boldsymbol{p}_{i-j} + \boldsymbol{u}^\top W_k^{\boldsymbol{e}} \boldsymbol{e}_j + \boldsymbol{v}^\top W_k^{\boldsymbol{r}} \boldsymbol{p}_{i-j}$$

Adding memory (aka "recurrence mechanism") (from Transformer-XL)

- ▶ When we have really large sequence, we can process it segment by segment
- ▶ When previous segment is processed, put it into cache and attend as embeddings like we do in machine translation



⁵And authors said that the model still underfit after 500K steps (but performance on downstream tasks didn't improve)



► How many TPUs v3 were used?

 $^{^5 \}mbox{And}$ authors said that the model still underfit after 500K steps (but performance on downstream tasks didn't improve)



▶ How many TPUs v3 were used? — 512

 $^{^5}$ And authors said that the model still underfit after 500K steps (but performance on downstream tasks didn't improve)



- ▶ How many TPUs v3 were used? 512
- ▶ How long did the thing trained?

 $^{^5}$ And authors said that the model still underfit after 500K steps (but performance on downstream tasks didn't improve)



- ▶ How many TPUs v3 were used? 512
- ► How long did the thing trained? 2.5 days⁵

 $^{^5}$ And authors said that the model still underfit after 500K steps (but performance on downstream tasks didn't improve)



- ▶ How many TPUs v3 were used? 512
- ► How long did the thing trained? 2.5 days⁵
- What was the batch size?

⁵And authors said that the model still underfit after 500K steps (but performance on downstream tasks didn't improve)

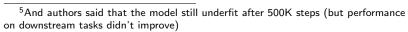


- ▶ How many TPUs v3 were used? 512
- ► How long did the thing trained? 2.5 days⁵
- ▶ What was the batch size? 2048

⁵And authors said that the model still underfit after 500K steps (but performance on downstream tasks didn't improve)



- ▶ How many TPUs v3 were used? 512
- ► How long did the thing trained? 2.5 days⁵
- ▶ What was the batch size? 2048
- What optimizer did they use?





- ▶ How many TPUs v3 were used? 512
- ► How long did the thing trained? 2.5 days⁵
- ▶ What was the batch size? 2048
- What optimizer did they use? Adam

⁵And authors said that the model still underfit after 500K steps (but performance on downstream tasks didn't improve)



TODO

I didn't have enough time to copy-paste tables from scores and ablation study, so let's open the paper and see them manually.



Things I didn't get

► Span-based prediction?

