CSE 493s/599s
Lecture 14. Transformers

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Lecture notes

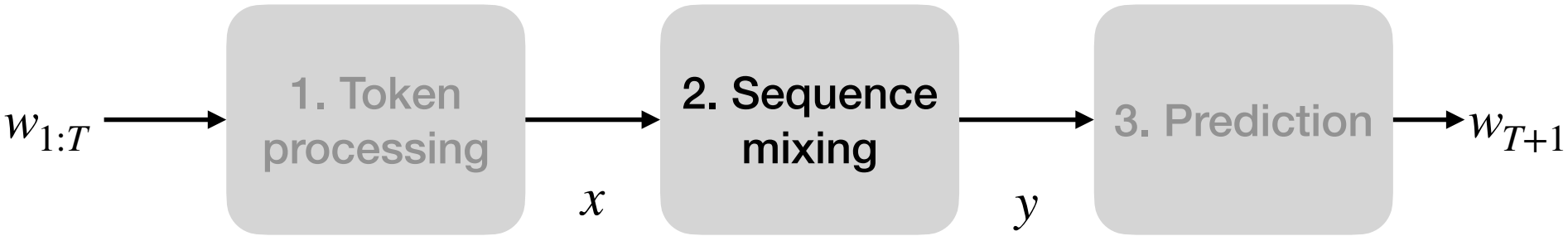
- These lecture notes are based on other courses in LLMs, including
  - CSE493S/599S at UW by Ludwig Schmidt: https://mlfoundations.github.io/advancedml-sp23/
  - EE-628 at EPFL by Volkan Cevher: https://www.epfl.ch/labs/lions/teaching/ee-628-training-large-language-models/ee-628-slides-2025/
  - ECE381V Generative Models at UT Austin by Sujay Sanghavi
  - and various papers and blogs cited at the end of the slide deck

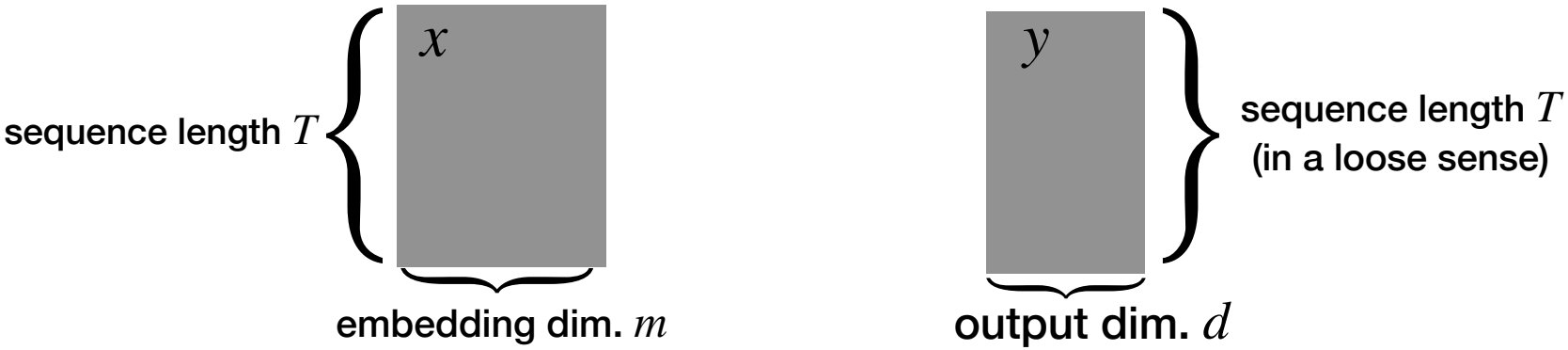
Outline

- Language models
- General LLM framework
  - Token processing
  - Sequence mixing
  - Prediction
- Example architectures

Sequence mixing

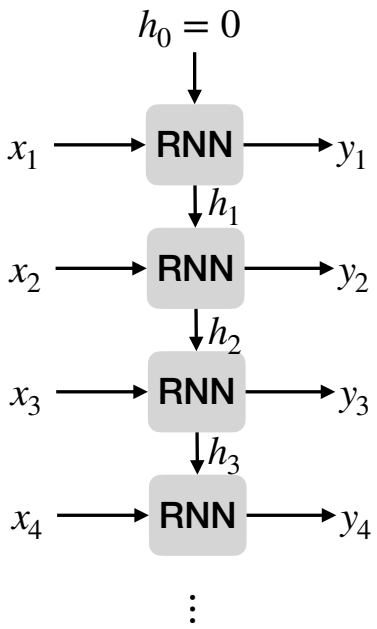
- Sequence mixing is one of the most well studied part of an LM that captures the dependencies across tokens.



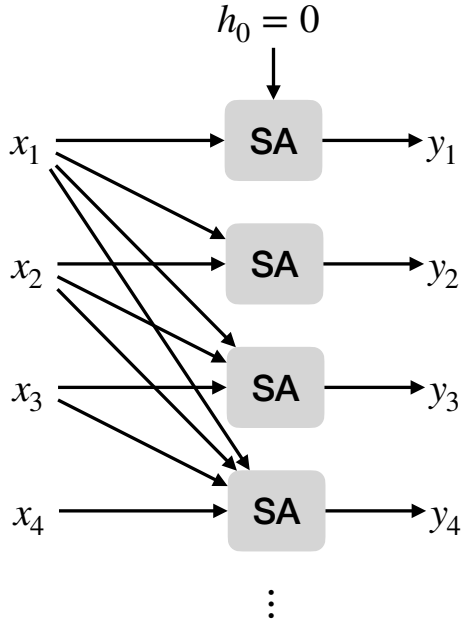


- **Self-attention** [Vaswani et al. 2017] as a sequence mixer addresses the shortcomings of RNNs with different trade-offs for inference cost.

RNNs are sequential

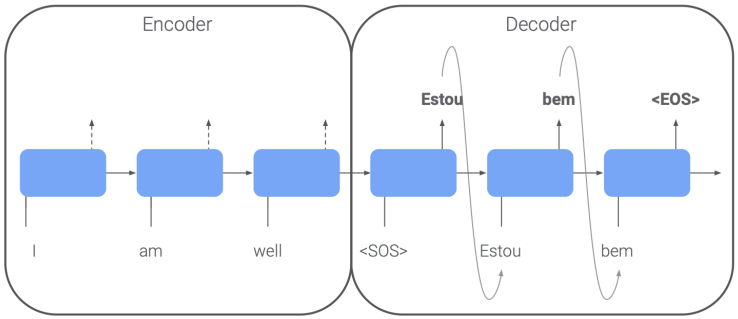


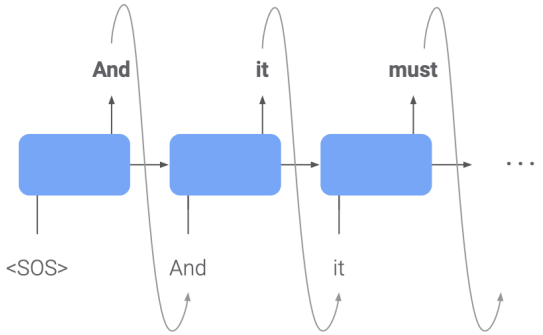
Self-attention is parallel



- Notice how we focus on a version of self-attention blocks that has a causal structure, i.e., the output only depends on the previous words. Both causal and non-causal are used depending on the application.

- Causal vs. non-causal dependencies determined by the user who chooses the architecture based on the application of interest.
- Original transformer paper was solving machine translation, where the “encoder” does not require causality, as its goal is to produce a vector representation of the entire sentence.

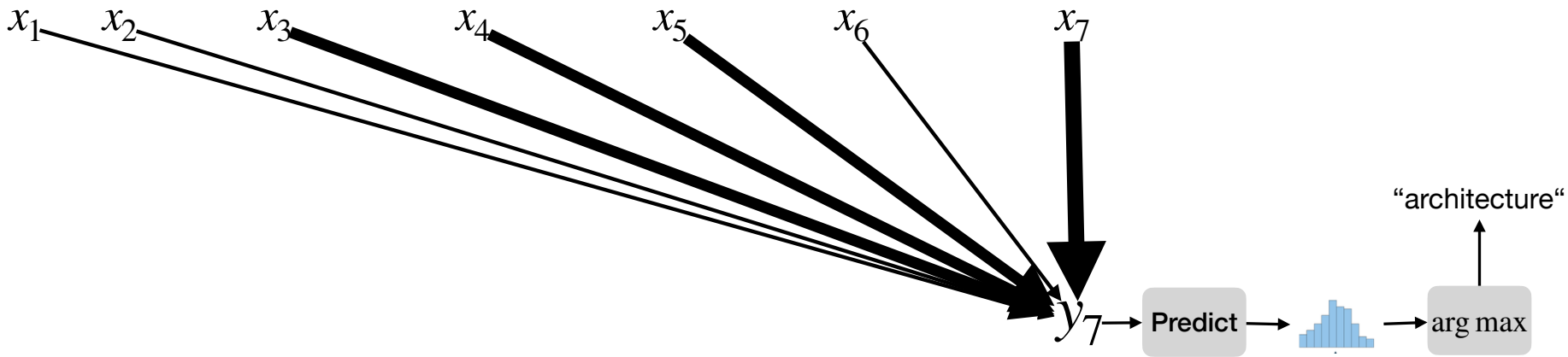




- Earlier language models, like BERT and RoBERTa, use what is called “masked” language model, where in training a random word is masked in a sentence and the model predicts it. Obviously, this is not causal and the transformer architecture used in these models is also not causal, i.e. a word in position i can attend to words both in the past and in the future.
- Modern LLMs, like GPT and Llama, are trained on next-word prediction tasks, which is obviously causal, since non-causal next-word prediction is a trivial. You just output the next token. As such, we focus in our lectures on causal structured self-attention mechanisms.

- The goal of a sequence mixer is to generate the representation of a word in a sequence that captures the true meaning of the word in the context the word is used in. For example,

  “To solve machine translation, Google introduced transformer architecture …”

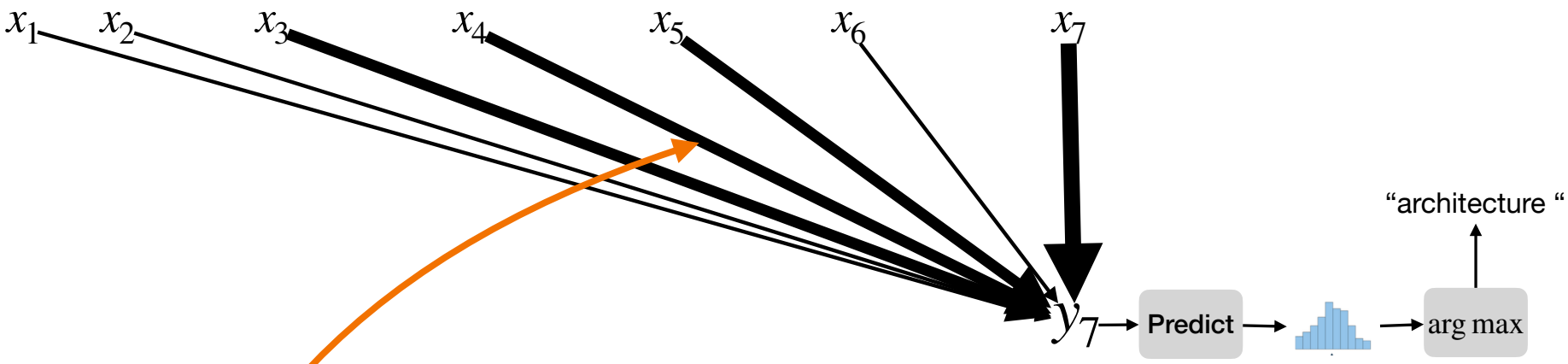


- Self-attention achieves this by a **weighted combination** of the vector embeddings of the other words, with more weight on a word that might be more relevant to the word of interest, say, “transformer”, i.e.,

$$y_t = c \cdot f(x_t) + \sum_{j \neq t} \alpha_{t;j} \cdot f(x_j) = \sum_{j=1}^{t} \alpha_{t;j} \cdot f(x_j)$$

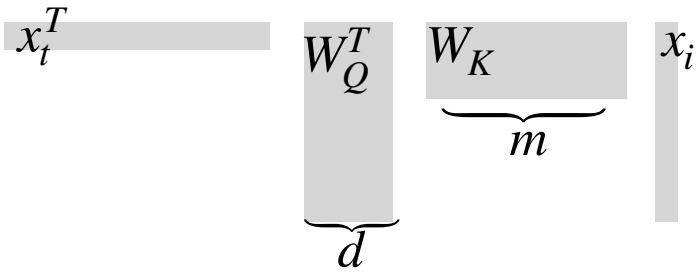
- Note that the relevance/weight $\alpha_{t;j}$ is asymmetric, since x_t is the target and x_j is the context.

- “To solve machine translation, Google introduced transformer …”



- To measure the similarity/relevance **key-query-value self-attention mechanism** uses **queries, keys, and values** with learnable parameters $W_Q, W_K, W_V \in \mathbb{R}^{d \times m}$. For modern language models, like GPT-4, the embedding dimension is $m = 12288$ and the query/key dimension is $d = 128$, such that the **query vector** for the target word is $q_t = W_Q x_t$, the **key vector** is $k_i = W_K x_i$, and the relevance is then

$$\text{Rel}(x_t; x_i) = \langle q_t, k_i \rangle = x_t^T W_Q^T W_K x_i$$



- $\mathrm{Rel}(x_t; x_i) = \langle q_t, k_i \rangle$ can be computed, for example, as a matrix, forcing upper-right triangle region to be $-\infty$, meaning no relevance, for **causality**. Output of self-attention can only depend on the past.

Query \ Key	To (x_1)	solve (x_2)	machine (x_3)	translation (x_4)	Google (x_5)	introduced (x_6)	transformer (x_7)
To	<q1,k1>						
solve	<q2,k1>	<q2,k2>					
machine	<q3,k1>	<q3,k2>	<q3,k3>				
translation	<q4,k1>	<q4,k2>	<q4,k3>	<q4,k4>			
Google	<q5,k1>	<q5,k2>	<q5,k3>	<q5,k4>	<q5,k5>		
introduced	<q6,k1>	<q6,k2>	<q6,k3>	<q6,k4>	<q6,k5>	<q6,k6>	
transformer	<q7,k1>	<q7,k2>	<q7,k3>	<q7,k4>	<q7,k5>	<q7,k6>	<q7,k7>
…							

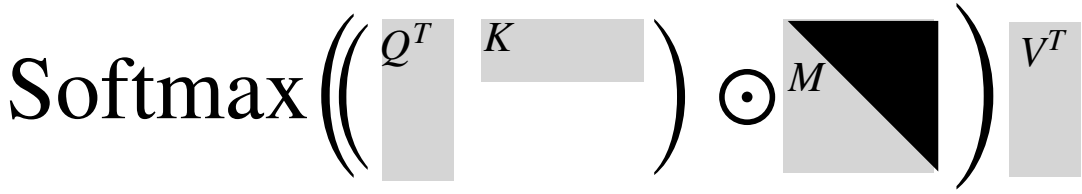
- $\langle q_{\text{transformer}}, k_{\text{Google}} \rangle$ might have a large positive value indicating that these terms are highly related, whereas $\langle q_{\text{transformer}}, k_{\text{to}} \rangle$ might be nearly zero or even negative.
- We would like to take the weighted sum of each row, to get a vector for the query word.

- For each column, we take the Softmax of the similarity to ensure that the weights are non-negative and sum to one, calling the previous Query-Key matrix Rel,

$$\alpha_{t;i} = \text{Softmax}(t\text{-th row of } \mathrm{Rel})_i = \mathrm{Softmax}(\{\langle q_t, k_j \rangle\}_{j=1}^{t})_i = \frac{e^{\langle q_t, k_i \rangle}}{\sum_{j=1}^{t} e^{\langle q_t, k_j \rangle}}$$

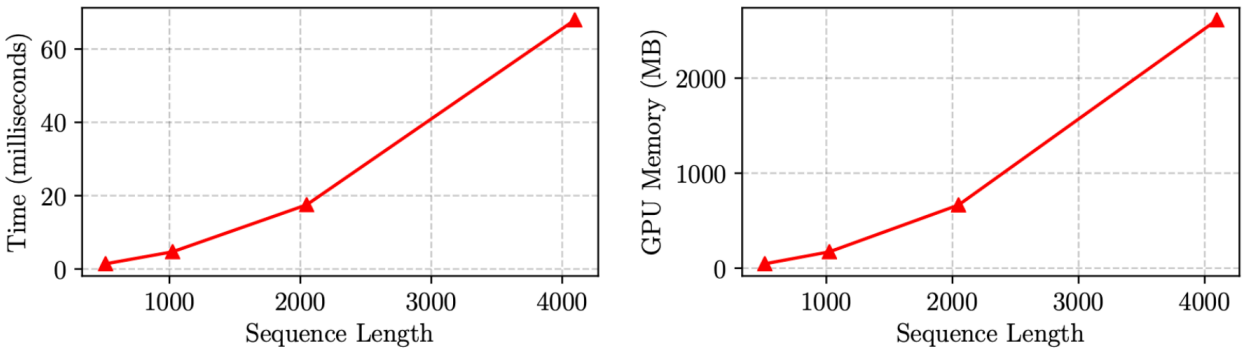
- The self-attention vector is the weighted sum of the **value** defined by a learnable parameter $W_V \in \mathbb{R}^{d \times m}$ such that $v_i = W_V x_i$, and

$$y_t = \sum_{i=1}^{t} \frac{e^{\langle q_t, k_i \rangle}}{\sum_{j=1}^{t} e^{\langle q_t, k_j \rangle}} v_i$$



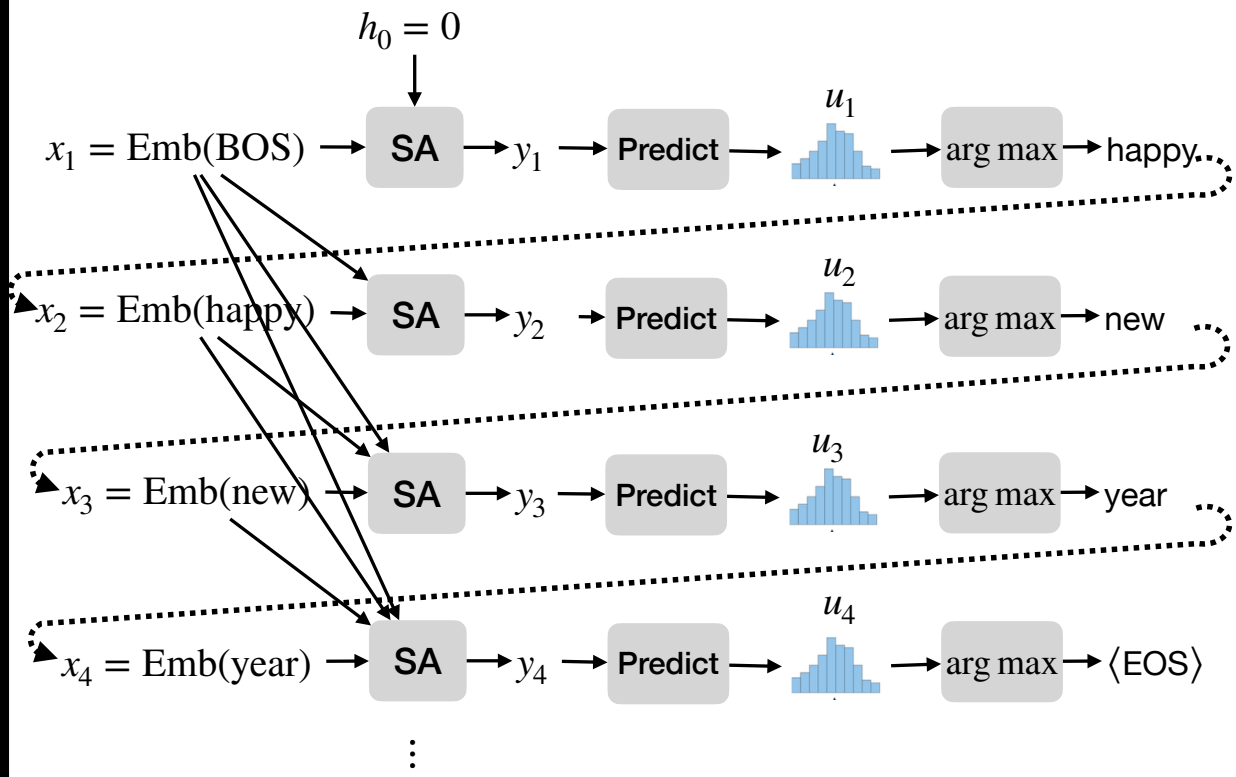
- All y_t's can be compactly represented as $Y = \mathrm{Softmax}((Q^T K) \odot M) V^T$, where $Q = \{q_i = W_Q x_i\}_{i=1}^{T} \in \mathbb{R}^{d \times T}$, $K = \{k_i = W_K x_i\}_{i=1}^{T} \in \mathbb{R}^{d \times T}$, $V = \{v_i = W_V x_i\}_{i=1}^{T} \in \mathbb{R}^{d \times T}$, and $M_{t,i} = \begin{cases} 1, & t \geq i \\ -\infty, & t < i \end{cases}$ is the causal mask.

- The causal mask is necessary in training, in order to prevent “cheating” in the next word prediction loss.
- Attention with masking is called **masked attention** or **causal attention**.
- By allowing any word to attend to any other word in the sequence, this resolves long-distance dependence problem of RNNs.
- Self-attention has learnable parameters: $W_Q, W_K, W_V \in \mathbb{R}^{d \times m}$.
- Note that the (masked) attention matrix is $T \times T$ dimension, and computation and memory scales like $O(T^2)$.



- Auto-regressive inference with self-attention

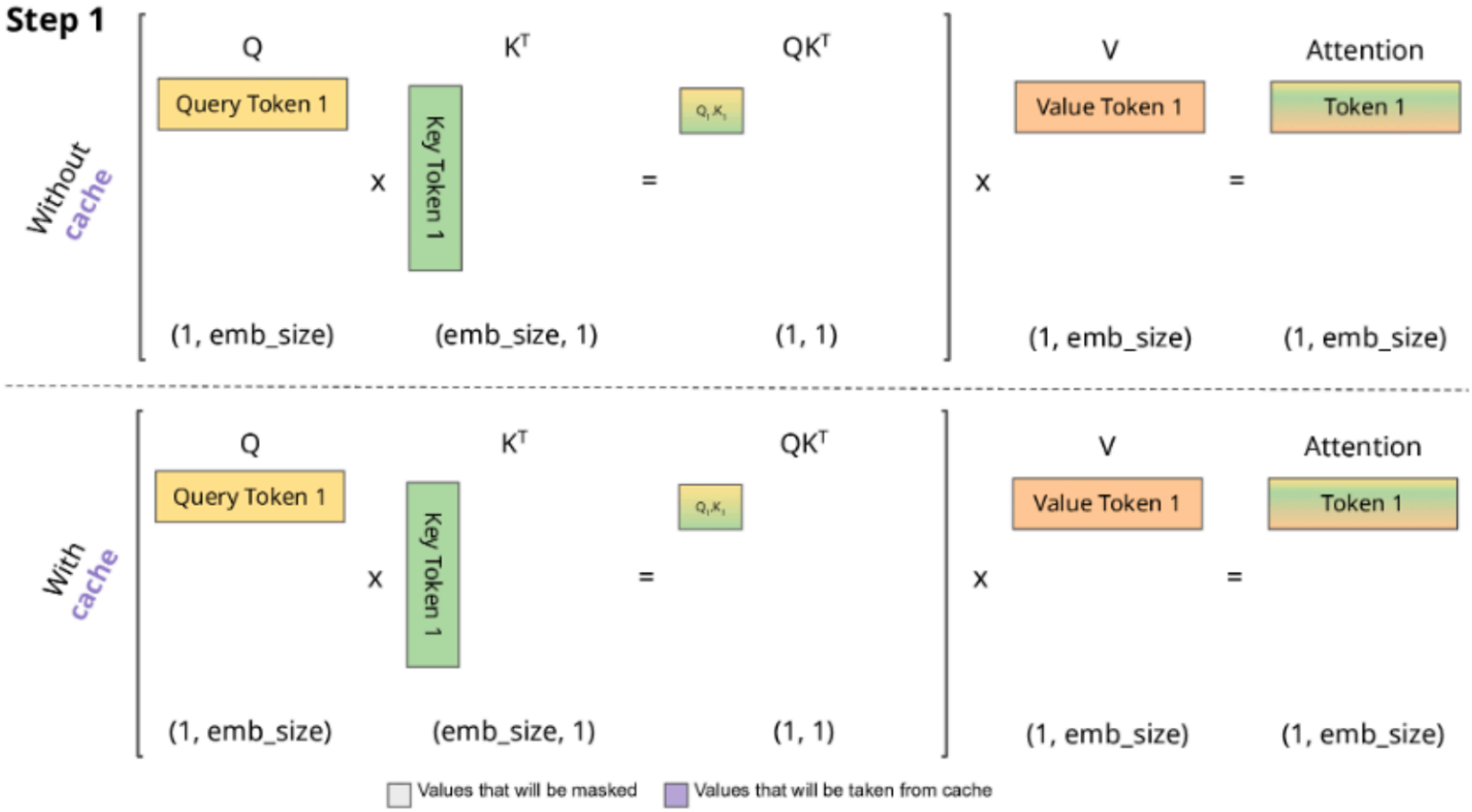
- Set x_1 as embedding of $\langle \text{BOS} \rangle$, t=1
- **While True:**
  - $q_t \leftarrow W_Q x_t, k_t \leftarrow W_K x_t, v_t \leftarrow W_V x_t$
  - compute score $s \leftarrow [q_t^T k_1, \cdots, q_t^T k_t,]^T$
  - $y_t \leftarrow [v_1, \cdots, v_t]\text{Softmax}(s)$
  - $x_{t+1} \leftarrow \text{Emb}(\arg\max_w u_t[w])$
  - If x_{t+1} is the embedding of $\langle \text{BOS} \rangle$: break
  - $t \leftarrow t + 1$
- **Output**: $[x_1, \cdots, x_{t+1}]$



- Note that this is still auto-regressive and non-parallelizable and hence slow, like RNN.

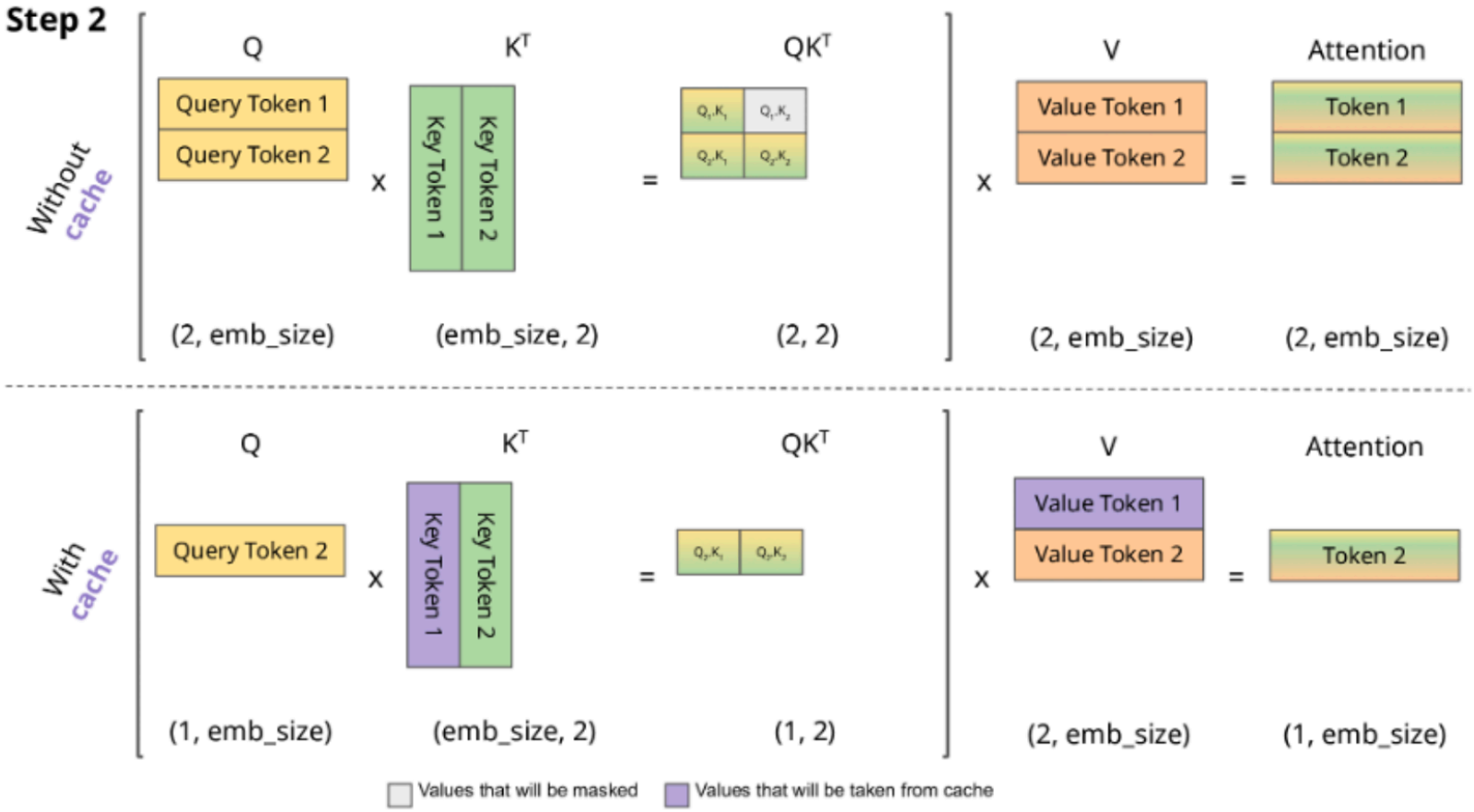
- How to speed up the computation of the attention heads is a very active research direction.
- **Definition** (KV cache)
  - **KV Cache** (Key-Value Cache) stores. computed keys (K) and values (V) from previous time steps to avoid recompilation in self-attention during autoregressive inference.
- How does KV Cache work?
  - $t = 1$: Compute and store k_1 and v_1.
  - $t = 2$: Retrieve k_1, v_1 and compute k_2, v_2 and append
  - for general t : retrieve all K, V and compute only key and value for the new word
- Naive implementation of self-attention recomputes K, V every step: $O(T^2 d)$.
- KV Cache reduces complexity to $O(Td)$ per step for faster **inference** with lower memory overhead. The idea is simple, and it is more about how to implement it in tensor operations. Training still takes $O(T^2 d)$ time.

- KV Cache



From https://medium.com/@joaolages/kv- caching- explained- 276520203249

- KV Cache



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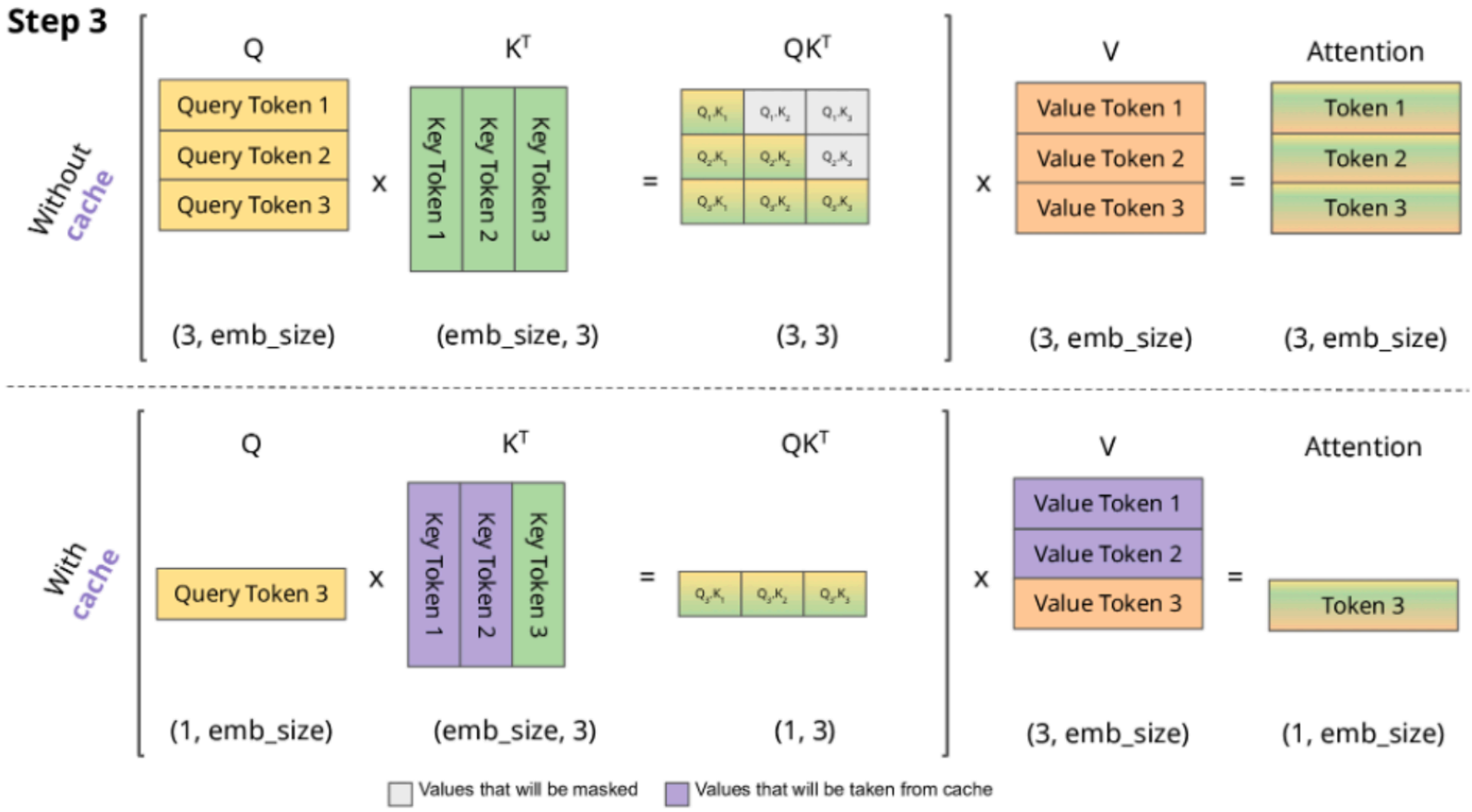
- KV Cache



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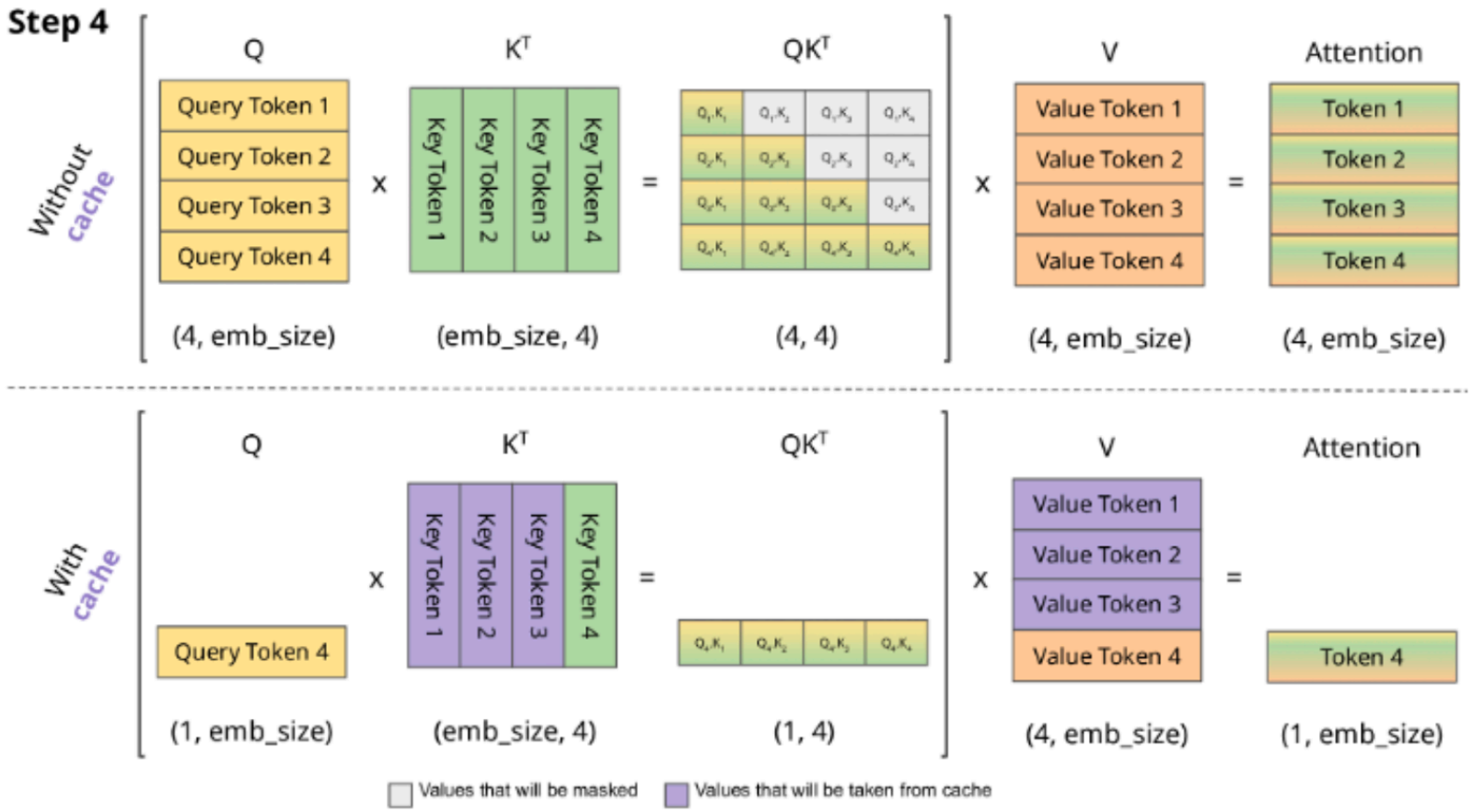
- KV Cache

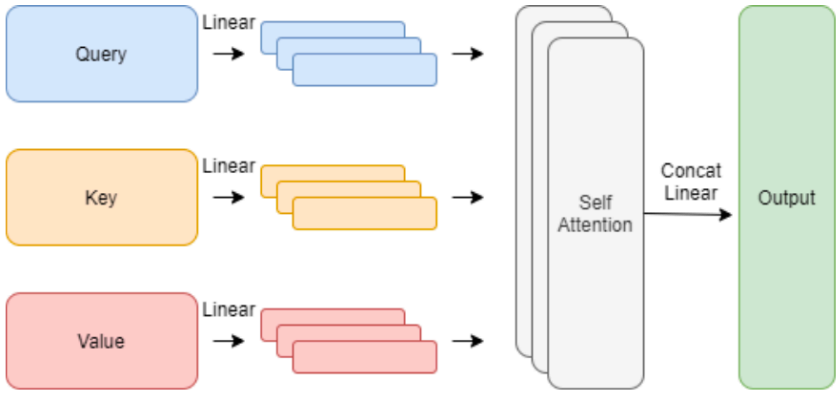


From https://medium.com/@joaolages/kv- caching- explained- 276520203249

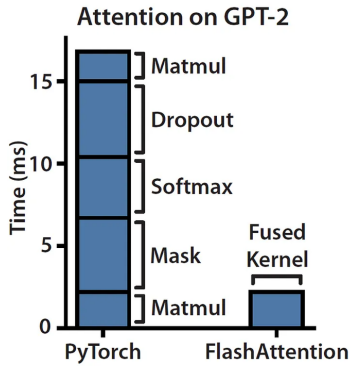
- Another idea to speed by parallelization is **multi-head attention.**
- **Definition** (Multi-head Attention)
  - Instead of having one attention, we can have h attention heads in parallel such that

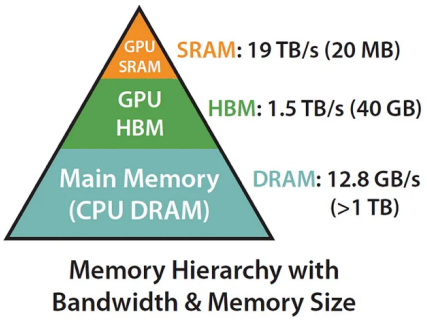
$$\text{MultiHead}(x) = \text{Concat}(\text{head}_1, \cdots, \text{head}_h),$$
$$\text{where } \text{head}_i = \text{Attention}\left(W_Q^{(i)}x, W_K^{(i)}x, W_V^{(i)}x\right).$$

- This division of heads allows parallelization.
- Each head handles different aspect, e.g., subject-verb agreement, syntax, semantic relations, etc, enhancing the model's ability to capture diverse dependencies.



- Matrix multiplications are **compute-bound**, i.e., run-time is dominated by computation, and element-wise operations are **memory-bound**, i.e., dominated by memory access
- Run-time of a transformer layer is dominated by Dropout, Softmax, Mask which are memory-bound.
- But memory is hierarchical. So the idea of **Flash attention** is to keep intermediate steps in SRAM (faster memory access) and only write the final result back to HBM (slower memory access).
- Use **tiling** to process in small blocks instead of full sequence.
- It is up to 2~4x faster with less memory footprint: $O(TCd)$ complexity where C is the size of the block.



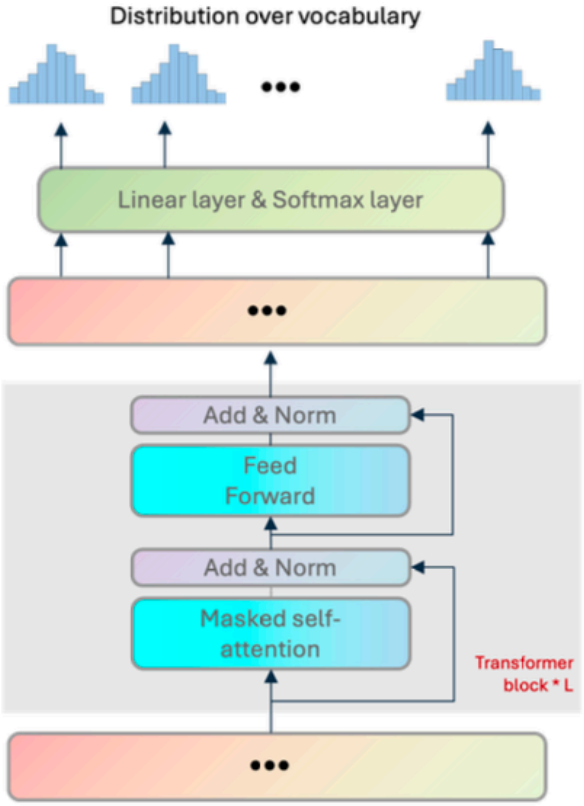


Memory Hierarchy with Bandwidth & Memory Size

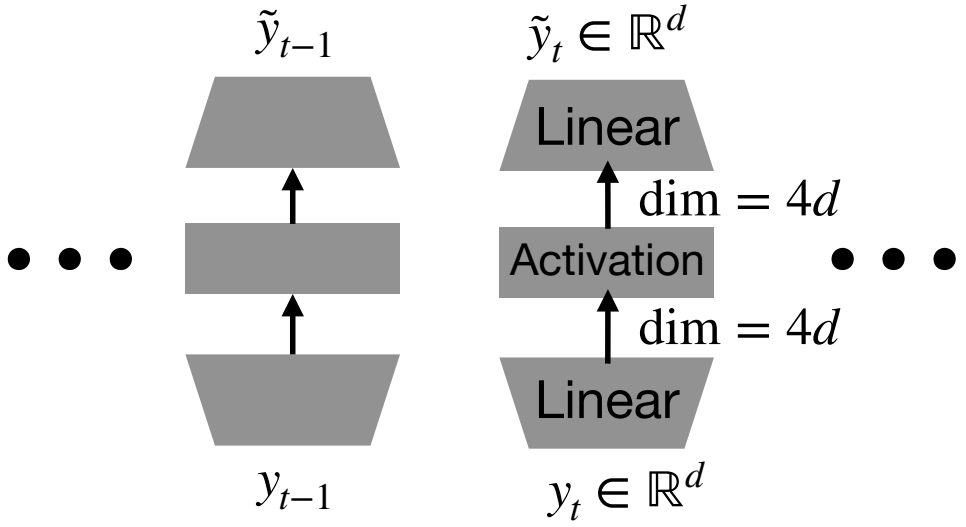
$$\text{Softmax}\left(\left(Q^T \quad K\right) \odot M\right) V^T$$

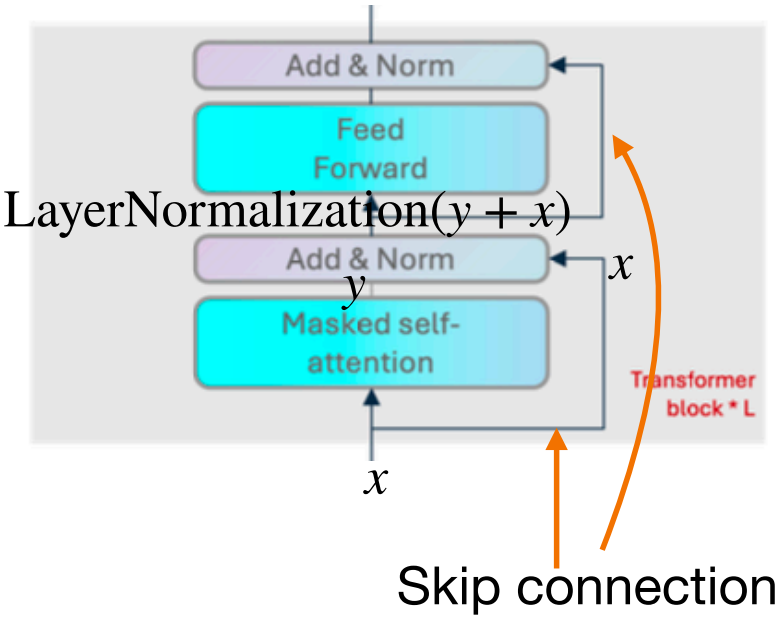
courtesy of https://gordicaleksa.medium.com/eli5-flash-attention-5c44017022ad

- Modern language models are made up of layers of transformer blocks.
- A transformer block is [self-attention + layer normalization + feedforward layer +layer normalization]
- GPT-2 has 12 heads and 12~48 layers.
- Original transformer is proposed with encoder and decoder for neural machine translation, but we only learned the transformer decoder which is sufficient as an LM.



- The role of **skip connection** is to prevent vanishing gradients (as we saw in the case of RNNs) by allowing gradients to flow directly from deeper layers to earlier layers.
    - It is motivated by ResNet's success in image classification.
- The role of **FFN** (applied to each token separately but shared weights) is to introduce additional non-linearity and improve expressiveness.

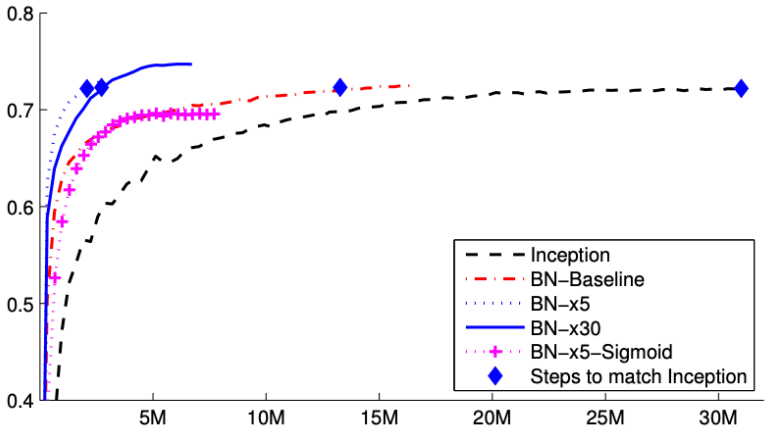




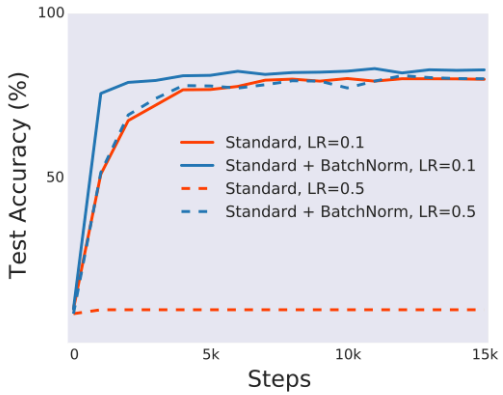
- To stabilize training, **Batch Normalization** and **Layer Normalization** are proposed.
- Batch normalization is initially proposed in [Ioffe et al. 2015] to mitigate a phenomena known as **internal covariate shift** by standardizing the input to each layer on the mini-batch that is being processed.
- **Covariate shift** is when the input distribution changes. **Internal covariate shift** is when the input distribution to a layer in a deep neural network changes, due to the sampling of a mini-batch.
- To mitigate such distribution changes, **batch normalization** standardizes the input to a layer: each input coordinate is subtracted its mini-batch mean and divided by the mini-batch standard deviation.
- This stabilizes the training, allowing larger step sizes and converging faster. At inference, moving average is used for the internal statistics.

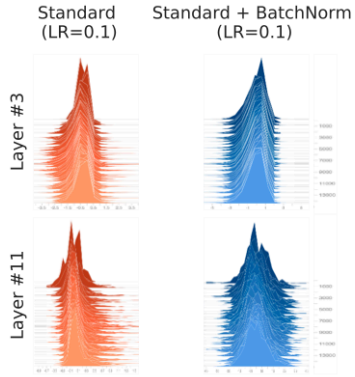
$$\mu_j = \frac{1}{B}\sum_{i=1}^{B} x_{i,j}, \sigma_j^2 = \frac{1}{B}\sum_{i=1}^{B}(x_{i,j} - \mu_j)^2$$

$$\tilde{x}_{i,j} = \frac{x_{i,j} - \mu_j}{\sqrt{\sigma_j^2 + \epsilon}}, \text{ for sample } i, \text{ coordinate } j$$



- One caveat is that the output of batch normalization is coordinate-wise scaled and shifted by learnable parameters, which we omit in the explanation.
- Later research [Santurkar et al. 2018] has discovered that the success of batch normalization has little to do with internal covariate shifts.





- Instead, batch normalization makes the **landscape smooth**, making it easier for gradient based optimization methods to take larger steps.
- However, for LLM training, each sample is processed separately, and hence batch size is oftentimes one. Further, sequence lengths are variable, so there is no predefined notion of a coordinate-wise statistics.

- **Layer normalization** [Ba et al. 2016] is similar but works with a single input sequence of arbitrary lengths.

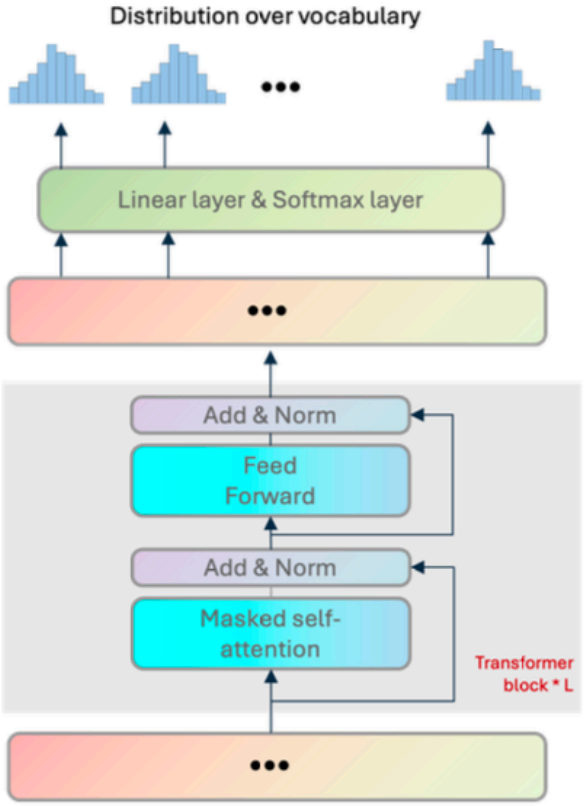
$$\mu_t = \frac{1}{d}\sum_{j=1}^{d} x_{t,j}, \sigma_t^2 = \frac{1}{d}\sum_{j=1}^{d}(x_{t,j} - \mu_t)^2$$

$$\tilde{x}_{t,i} = \frac{x_{t,i} - \mu_t}{\sqrt{\sigma_t^2 + \epsilon}}, \text{ for position } t, \text{ coordinate } i$$

- This is widely used in LLMs' transformer layers to stabilize the training dynamics.

- Forward pass in pre-training on single sentence:

  - Initial loss $L = 0$, and let $y_0 = x$
  - For each layer $\ell = 1, \ldots, \mathscr{L}$
    - $Q_\ell \leftarrow W_{Q,\ell} y_{\ell-1}$, $K_\ell \leftarrow W_{K,\ell} y_{\ell-1}$, $V_\ell \leftarrow W_{V,\ell} y_{\ell-1}$
    - $S_\ell \leftarrow \text{Mask}(Q_\ell^T K_\ell)$
    - $y_\ell \leftarrow \text{Row-wise-Softmax}(S_\ell) V_\ell^T$
    - $y_\ell \leftarrow \text{Layernorm}(y_\ell + y_{\ell-1})$
    - $y_{\text{skip}} \leftarrow y_\ell$
    - $y_\ell \leftarrow W_{F2,\ell}\, \sigma(W_{F1,\ell} y_\ell)$
    - $y_\ell \leftarrow \text{Layernorm}(y_\ell + y_{\text{skip}})$
  - $u = [u_1, \ldots, u_T] \leftarrow \text{Row-wise-Softmax}(W_O y_{\mathscr{L}})$
  - $L += \left(\sum_{t=1}^{T} \sum_{i=1}^{|\mathscr{V}|} -\hat{u}_t^{(i)} \log(u_t^{[i]}) \right)$



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  - Sequence mixing
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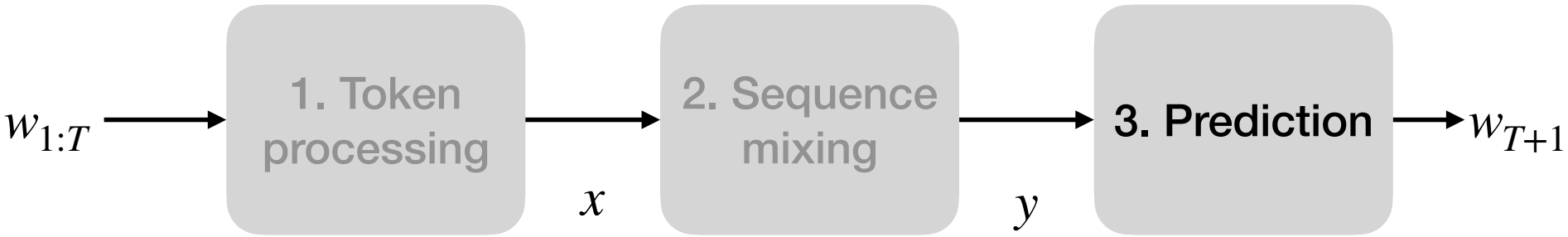
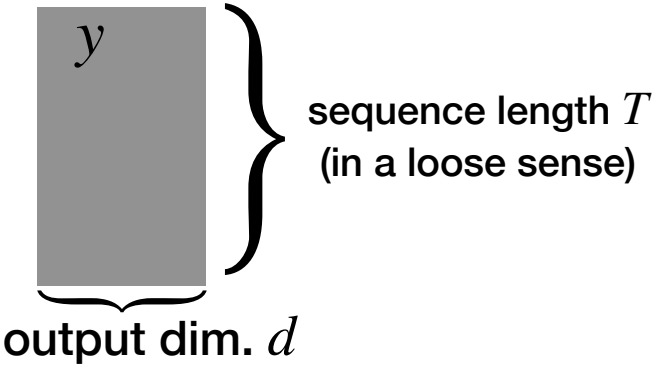
- Example architectures

Prediction

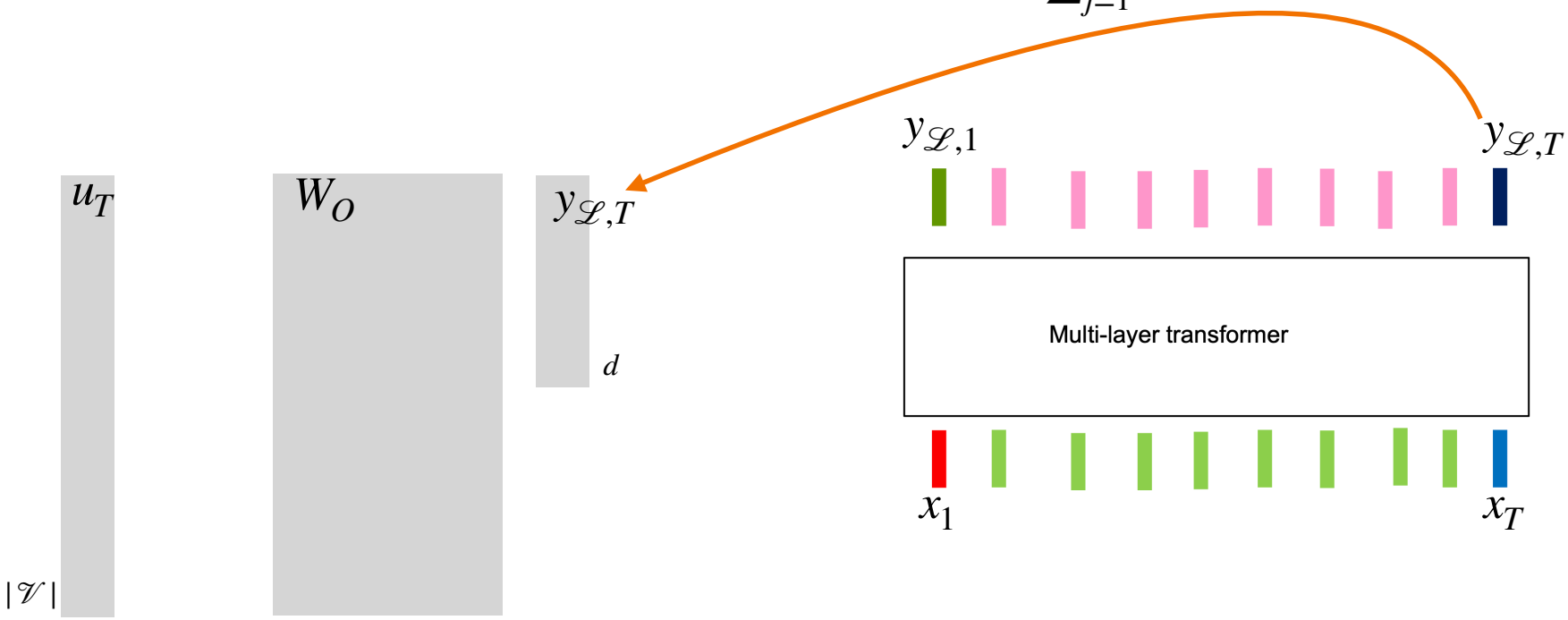
- Next token prediction involve outputting a distribution over the vocab and sampling from the distribution.



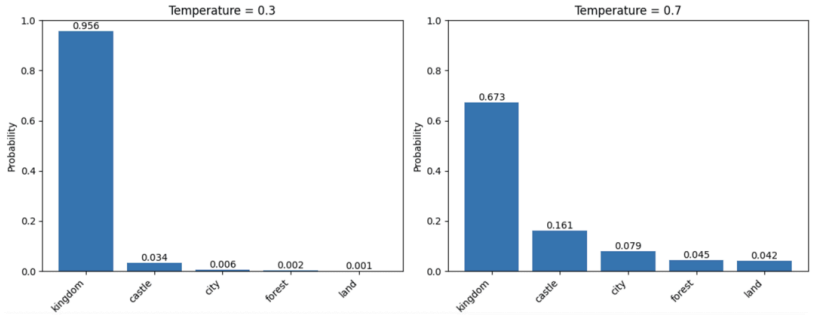


- The last transformer block outputs $y_{\mathscr{L}} \in \mathbb{R}^{T \times d}$.
- The prediction layer takes the output representation of the last word, $y_{\mathscr{L},T}$, to predict the next token, with a learnable parameter $W_O \in \mathbb{R}^{|\mathscr{V}| \times d}$, which may or may not be sharing weights with the input token embedding matrix.

$$u_T \leftarrow \text{Softmax}(W_O y_{\mathscr{L},T}) \qquad u_{T,i} = \mathbb{P}(i\text{-th token}) = \frac{e^{W_{O,i} y_{\mathscr{L},t}}}{\sum_{j=1}^{|\mathscr{V}|} e^{W_{O,j} y_{\mathscr{L},t}}}$$



- Given the token distribution, there are many ways to sample tokens, auto-regressively.
  - Auto-regressive sampling uses the chain rule to break the distribution on the sentence into:
    $$\mathbb{P}(S) = \mathbb{P}(w_{1:T}) = \mathbb{P}(w_1)\mathbb{P}(w_2 \mid w_1)\mathbb{P}(w_3 \mid w_1, w_2)\cdots\mathbb{P}(w_T \mid w_{1:T-1})$$
    - If the LM predicts an accurate and **calibrated *conditional distribution***, then random sampling auto-regressively provides an exact sample from the ***joint distribution*** on the sentence:
      Random sampling samples a token from the distribution u_t, each time until <EOS>, but can generate out-of-distribution samples, resulting in hallucination and non-grammatical sentences.
      LMs are not well calibrated since they are trained as classifiers with cross-entropy.
  - On the other extreme is **Greedy sampling,** which samples the highest probability token, deterministically.
  - In practice, one balances the two ends by **Sampling with temperature** T, usually between 0 and 1, which samples from an adjusted Softmax($W_O y_{\mathscr{L},t}$):
    $$u_{t,i} = \mathbb{P}(i\text{-th token}) = \frac{e^{W_{O,i} y_{\mathscr{L},t}/T}}{\sum_{j=1}^{|\mathscr{V}|} e^{W_{O,j} y_{\mathscr{L},t}/T}},$$
    where $T = 1$ recovers the original random sampling,
    T=0 recovers the greedy sampling,
    0<T<1 balances the two.
    T is tuned like a hyper-parameter at inference time.



Next-word probabilities under different temperatures

  - **Top-k sampling** samples from u_t but only among the top-k tokens.
  - **Nucleus sampling** (also known as top-p sampling) [Holtzman et al. 2020] samples from u_t but only among the smallest set whose cumulative probability exceeds $p \in (0,1)$

- **Greedy sampling** attempts to solve

$$\arg\max_{w_{1:T}} \mathbb{P}(w_{1:T}) \approx \arg\max_{w_1} \mathbb{P}(w_1) \arg\max_{w_2} \mathbb{P}(w_2 \mid w_1^*) \mathbb{P} \cdots \arg\max_{w_T} \mathbb{P}(w_T \mid w_{1:T-1}^*),$$

  where w_t^*'s are the solution of the previous maximization.

- Instead, we can try to better approximate the most likely sequence directly (solving the LHS of above), using **Beam search,** which produces high quality but low-diversity sequences.

- (deterministic) Beam search with beam width B proceeds as follows.

  - B most likely candidates are selected for the first token.
  - For each token at position 1, k most likely next tokens are selected.
  - Out of kB candidates for a sequence of length 2, the most likely B candidates are chosen.
  - This repeats until B candidates end on <EOS>.

Context: In a shocking finding, scientist discovered a herd of unicorns living in a remote, previously unexplored valley, in the Andes Mountains. Even more surprising to the researchers was the fact that the unicorns spoke perfect English.

Beam Search, *b*=32:
"The study, published in the Proceedings of the National Academy of Sciences of the United States of America (PNAS), was conducted by researchers from the Universidad Nacional Autónoma de México (UNAM) and the Universidad Nacional Autónoma de México (UNAM/Universidad Nacional Autónoma de México/Universidad Nacional Autónoma de México/Universidad Nacional Autónoma de México/Universidad Nacional Autónoma de ..."

Pure Sampling:
They were cattle called Bolivian Cavalleros; they live in a remote desert uninterrupted by town, and they speak huge, beautiful, paradisiacal Bolivian linguistic thing. They say, 'Lunch, marge.' They don't tell what the lunch is," director Professor Chuperas Omwell told Sky News. "They've only been talking to scientists, like we're being interviewed by TV reporters. We don't even stick around to be interviewed by TV reporters. Maybe that's how they figured out that they're cosplaying as the Bolivian Cavalleros."

Figure 1: Even with substantial human context and the powerful GPT-2 Large language model, Beam Search (size 32) leads to degenerate repetition (highlighted in blue) while pure sampling leads to incoherent gibberish (highlighted in red). When $b \geq 64$, both GPT-2 Large and XL (774M and 1542M parameters, respectively) prefer to stop generating immediately after the given context.

In practice, **Nucleus sampling** strikes the right balance and usually performs the best.

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