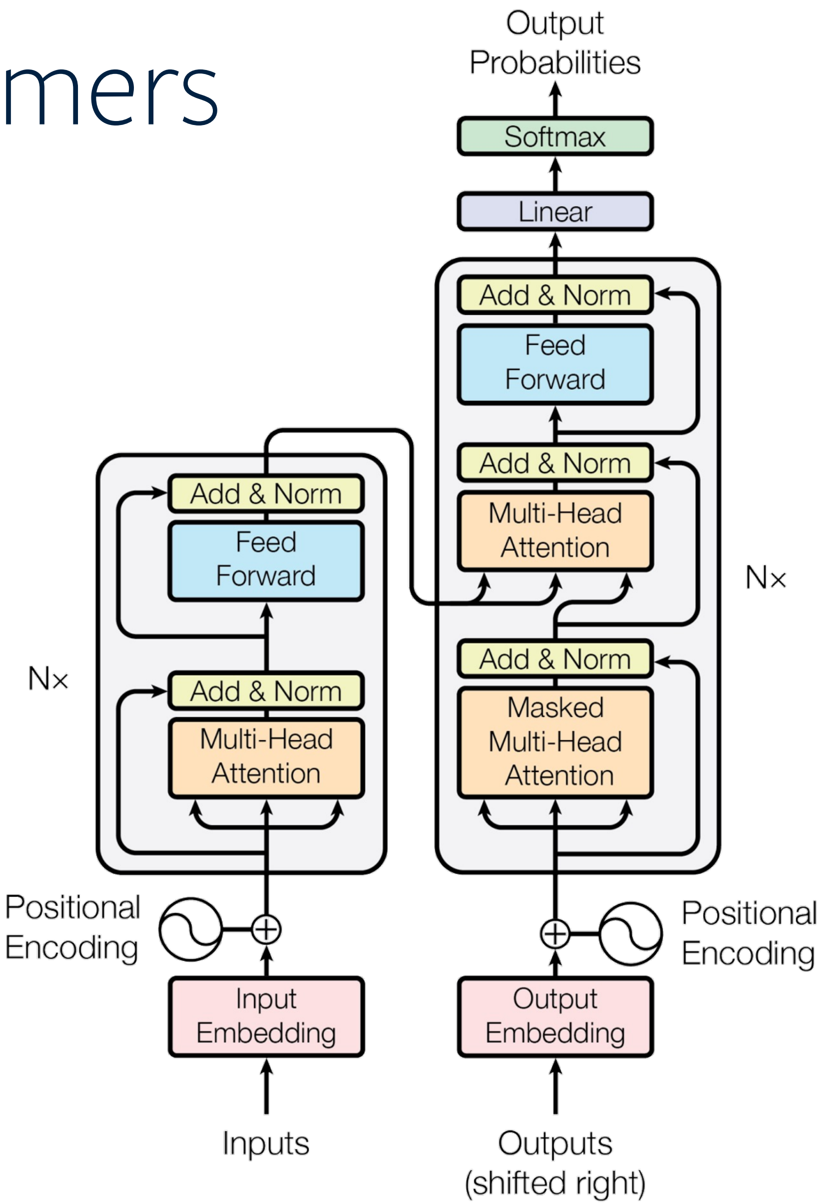
Scan and Snap: Understanding Training Dynamics and Token Composition in 1-layer Transformer

Yuandong Tian[1] Yiping Wang[2,4] Beidi Chen[1,3] Simon Du[2]

[1]Meta AI (FAIR) [2]University of Washington [3]Carnegie Mellon University [4]Zhejiang University

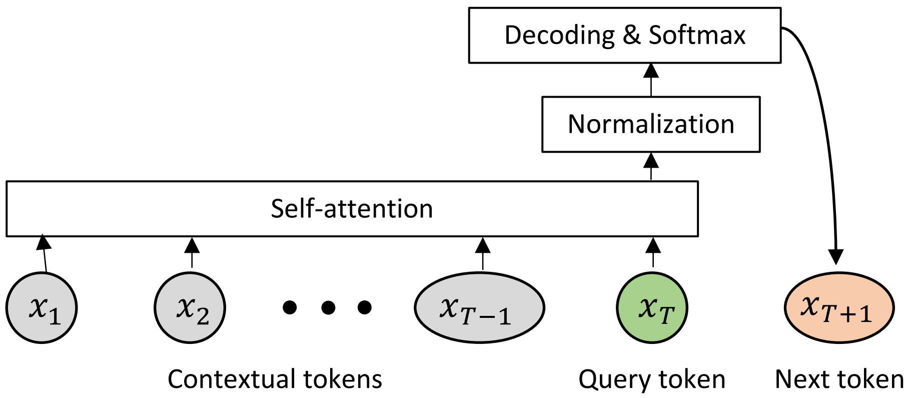
Transformers



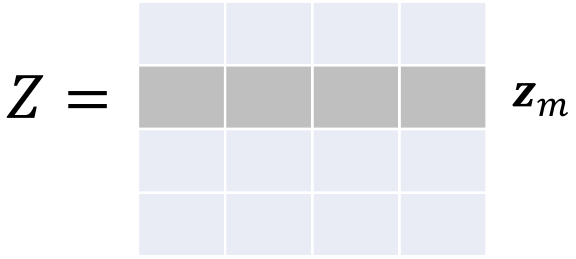
[A. Vaswani et al, Attention is all you need, NeurIPS'17]

Why it works?

Problem Settings



- Reparameterization
  - $Y = UW_V^T U^T$
  - $Z = UW_Q W_K^T U^T$ (pairwise logits of self-attention matrix)



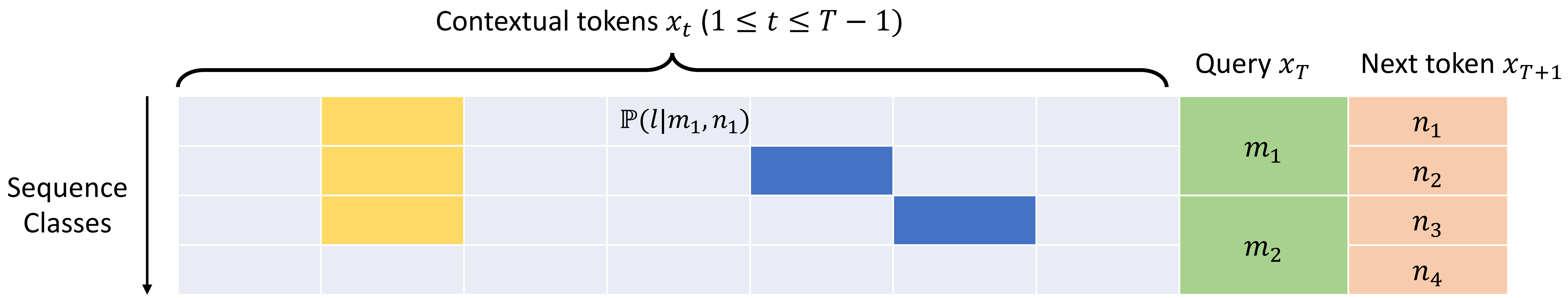
$\boldsymbol{z}_m$: All logits of the contextual tokens when attending to last token $x_T = m$

- Assumptions
  - No positional encoding
  - Sequence length $T \to +\infty$
  - Learning rate of decoder Y larger than self-attn layer Z ($\eta_Y \gg \eta_Z$)

- Other technical assumptions

Data Distribution

$x_t \in [M]$ for $1 \le t \le T$
$x_{T+1} \in [K]$
$K \ll M$



Distinct tokens: There exists unique n so that $\mathbb{P}(l|n) > 0$

Common tokens: There exists multiple n so that $\mathbb{P}(l|n) > 0$

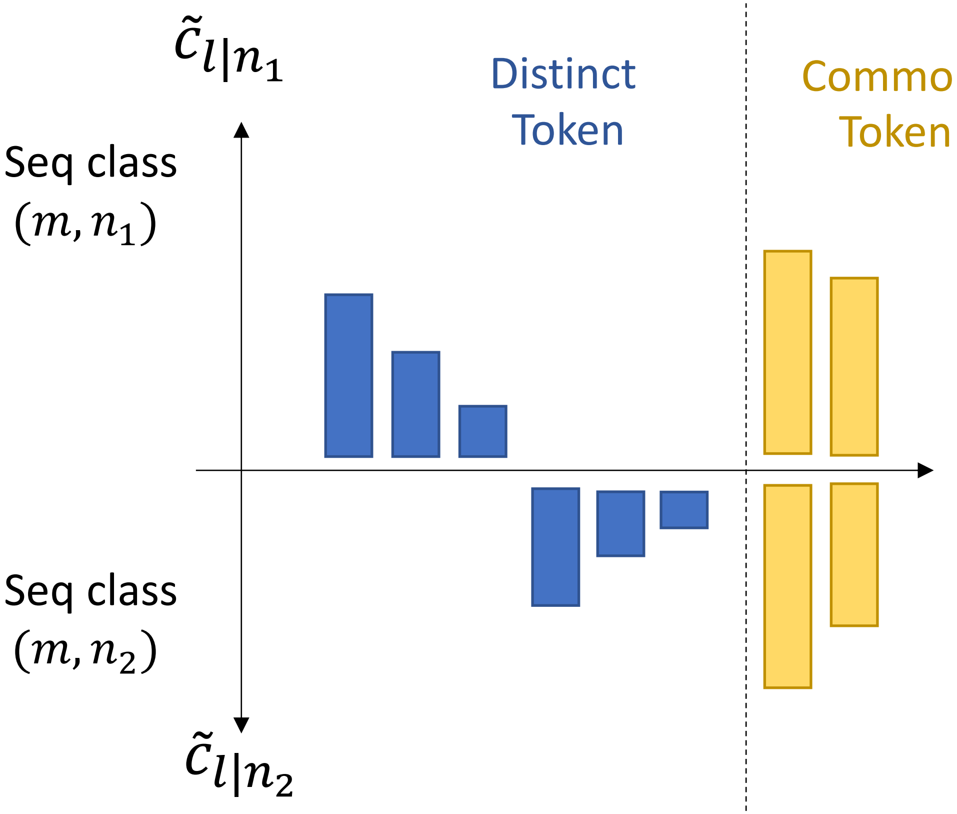
$\mathbb{P}(l|m,n) = \mathbb{P}(l|n)$ is the conditional probability of token l given last token $x_T = m$ and $x_{T+1} = n$

Assumption: $m = \psi(n)$, i.e., no next token shared among different last tokens

Question: Given the data distribution, how does the self-attention layer behave?

Overall Picture of the Training Dynamics

<u>At initialization</u>



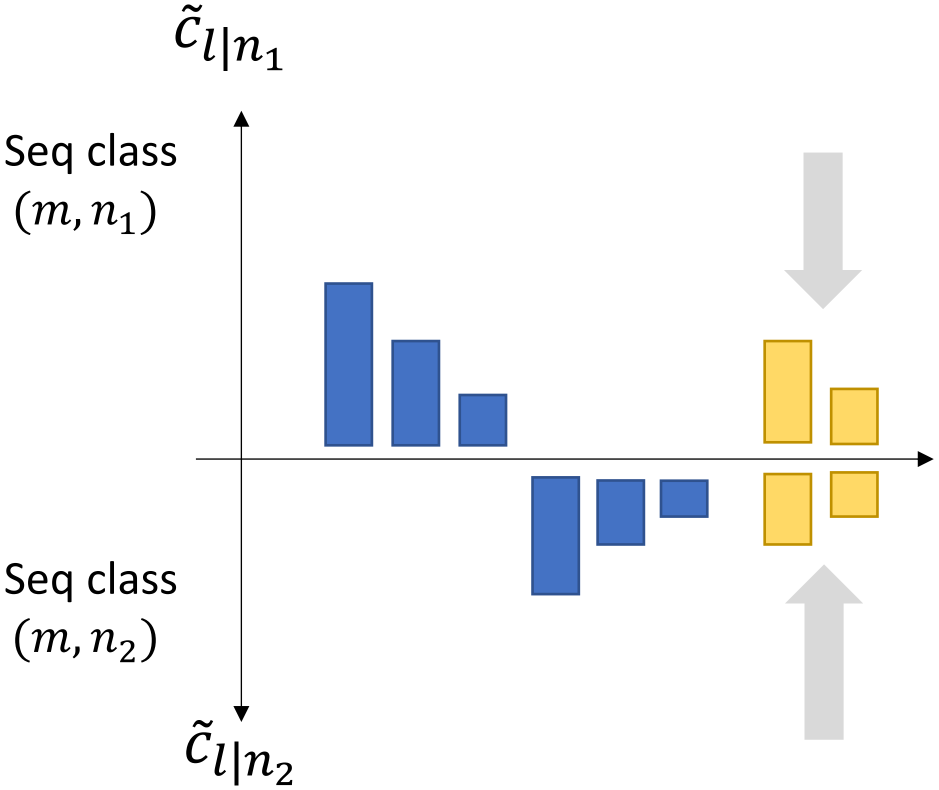
Co-occurrence probability

$$\tilde{c}_{l|n_1} := \mathbb{P}(l|m, n_1)\exp(z_{ml})$$

Initial condition: $z_{ml}(0) = 0$

Overall Picture of the Training Dynamics

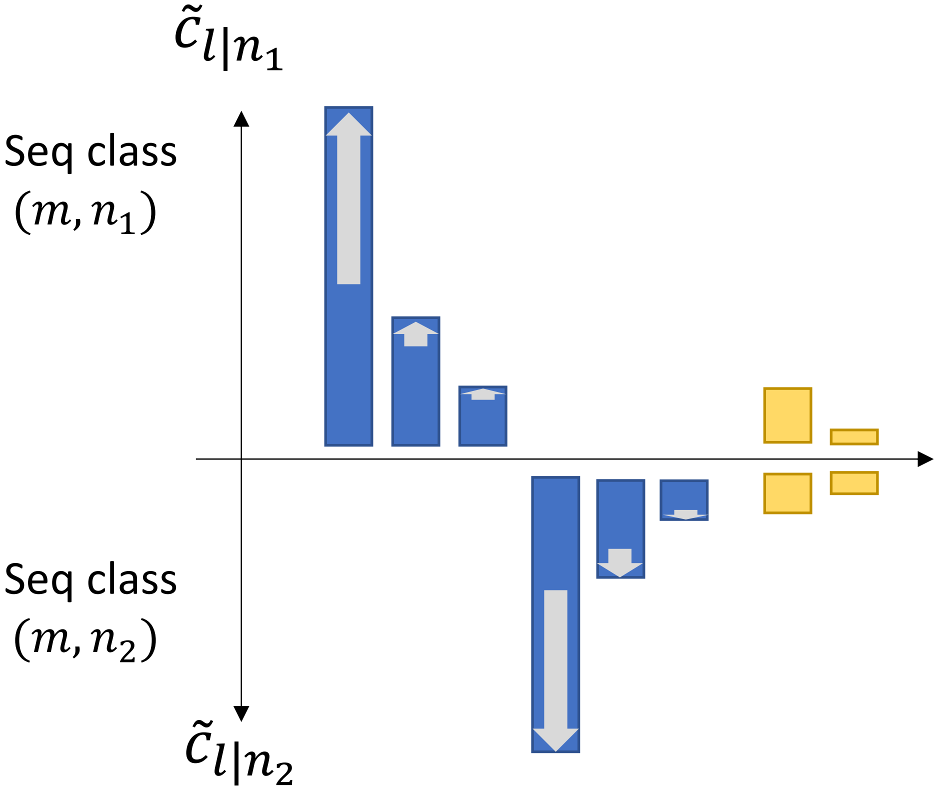
Common Token Suppression



(a) $\dot{z}_{ml} < 0$, for common token l

Overall Picture of the Training Dynamics

Winners-emergence



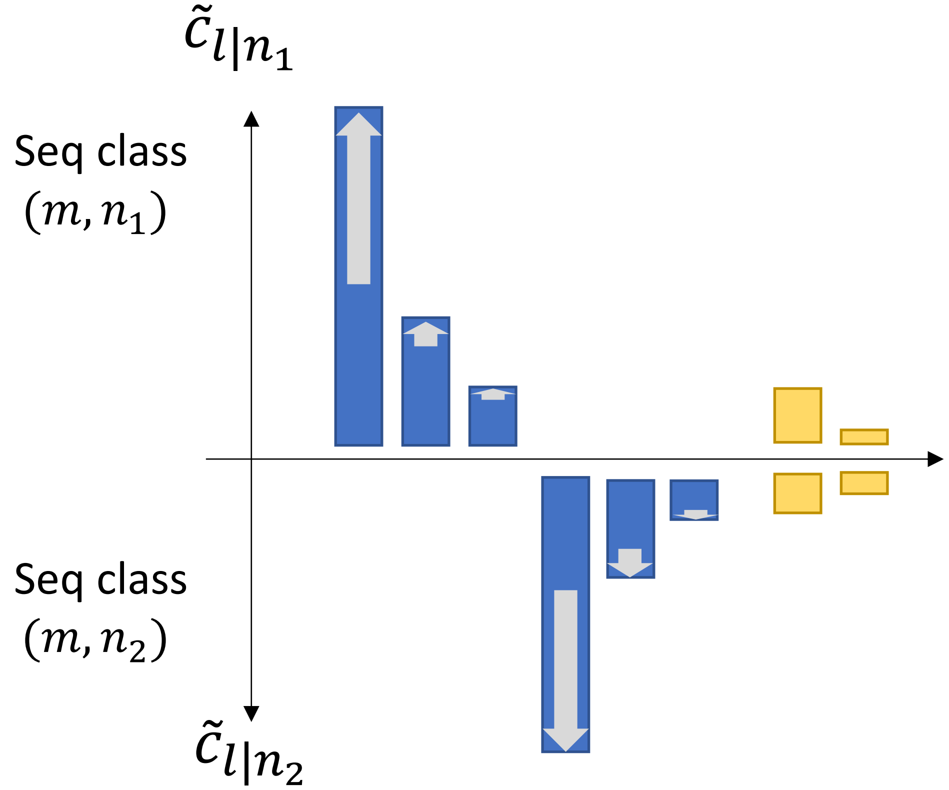
(a) $\dot{z}_{ml} < 0$, for common token l

(b) $\dot{z}_{ml} > 0$, for distinct token l

Learnable TF-IDF (Term Frequency, Inverse Document Frequency)

Overall Picture of the Training Dynamics

Winners-emergence



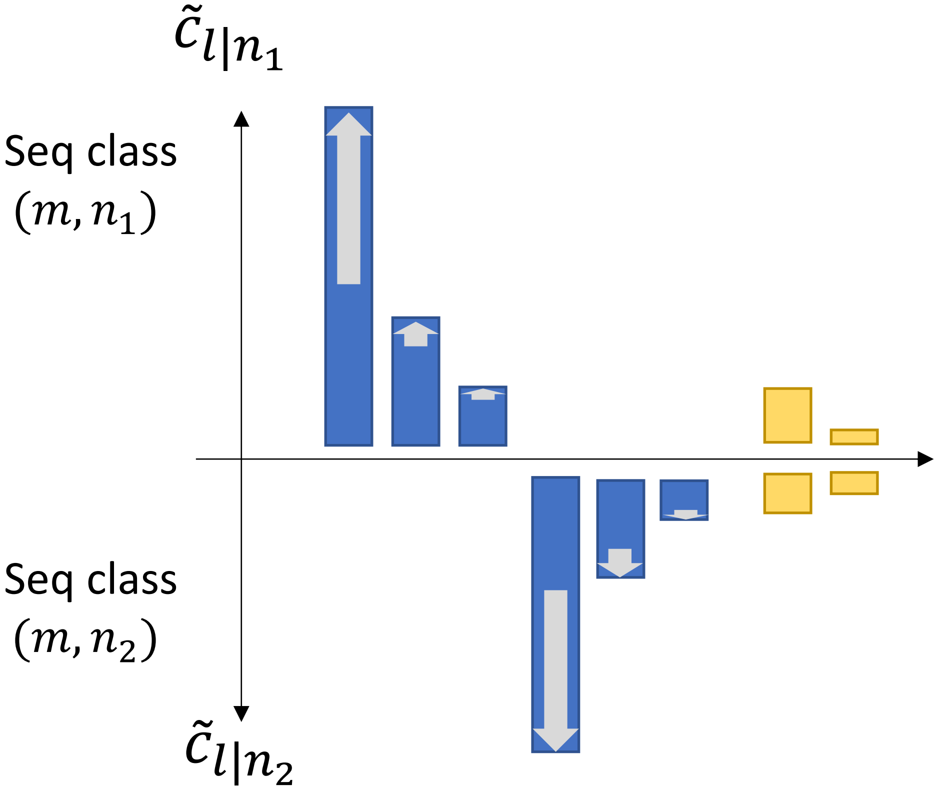
(a) $\dot{z}_{ml} < 0$, for common token l

(b) $\dot{z}_{ml} > 0$, for distinct token l

(c) $z_{ml}(t)$ grows faster with larger $\mathbb{P}(l|m, n)$

Overall Picture of the Training Dynamics

Winners-emergence



(c) $z_{ml}(t)$ grows faster with larger $\mathbb{P}(l|m,n)$

Theorem 3 Relative gain $r_{l/l'|n}(t) := \frac{\tilde{c}^2_{l|n}(t)}{\tilde{c}^2_{l'|n}(t)} - 1$ has a close form:

$$r_{l/l'|n}(t) = r_{l/l'|n}(0)\chi_l(t)$$

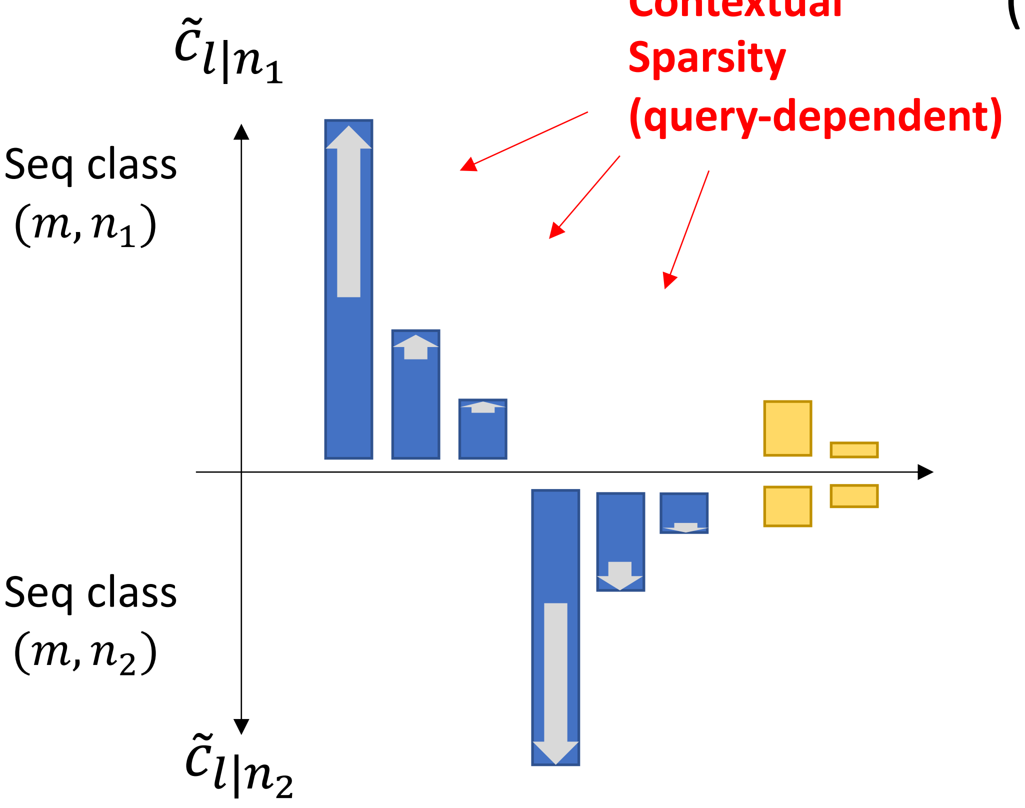
If l_0 is the dominant token: $r_{l_0/l|n}(0) > 0$ for all $l \neq l_0$ then

$$e^{2f^2_{nl_0}(0)B_n(t)} \leq \chi_{l_0}(t) \leq e^{2B_n(t)}$$

where $B_n(t) \geq 0$ monotonously increases, $B_n(0) = 0$

Overall Picture of the Training Dynamics

Winners-emergence



(c) $z_{ml}(t)$ grows faster with larger $\mathbb{P}(l|m,n)$

Theorem 3 Relative gain $r_{l/l'|n}(t) := \frac{\tilde{c}^2_{l|n}(t)}{\tilde{c}^2_{l'|n}(t)} - 1$ has a close form:

$$r_{l/l'|n}(t) = r_{l/l'|n}(0)\chi_l(t)$$

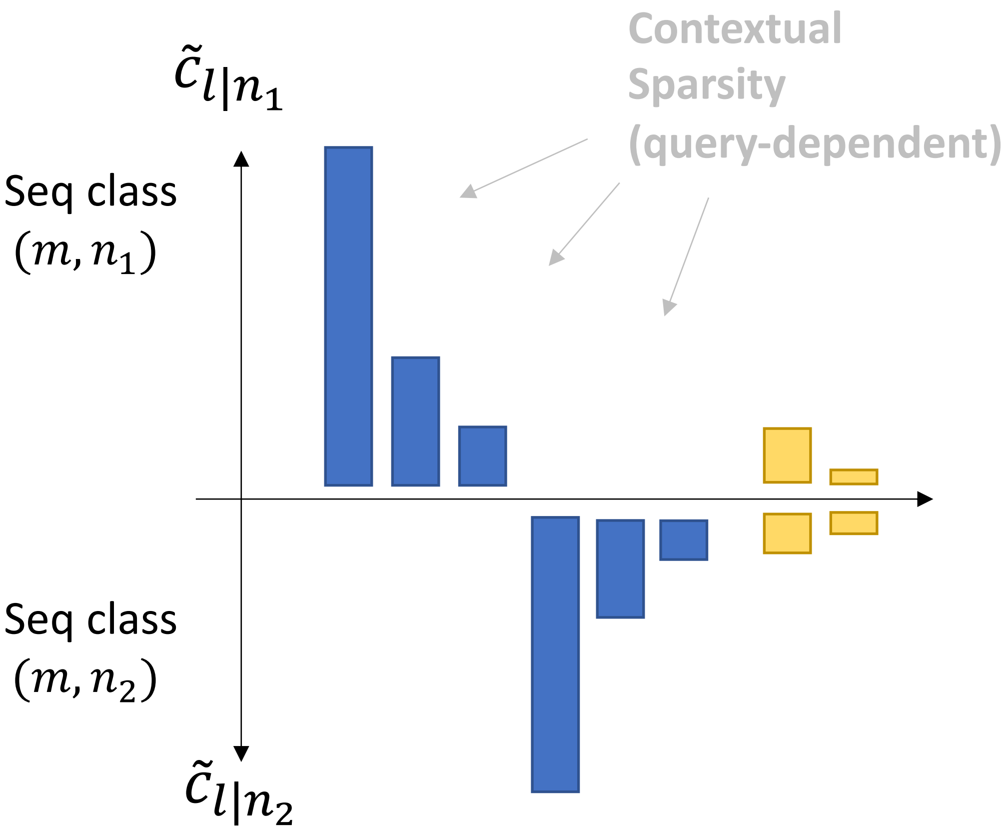
If l_0 is the dominant token: $r_{l_0/l|n}(0) > 0$ for all $l \neq l_0$ then

$$e^{2f^2_{nl_0}(0)B_n(t)} \leq \chi_{l_0}(t) \leq e^{2B_n(t)}$$

where $B_n(t) \geq 0$ monotonously increases, $B_n(0) = 0$

Overall Picture of the Training Dynamics

Attention frozen



Theorem 4 When $t \to +\infty$,

$$B_n(t) \sim \ln\left(C_0 + 2K\frac{\eta_Z}{\eta_Y}\ln^2\left(\frac{M\eta_Y t}{K}\right)\right)$$

Attention **scanning**:

When training starts, $B_n(t) = O(\ln t)$

Attention **snapping**:

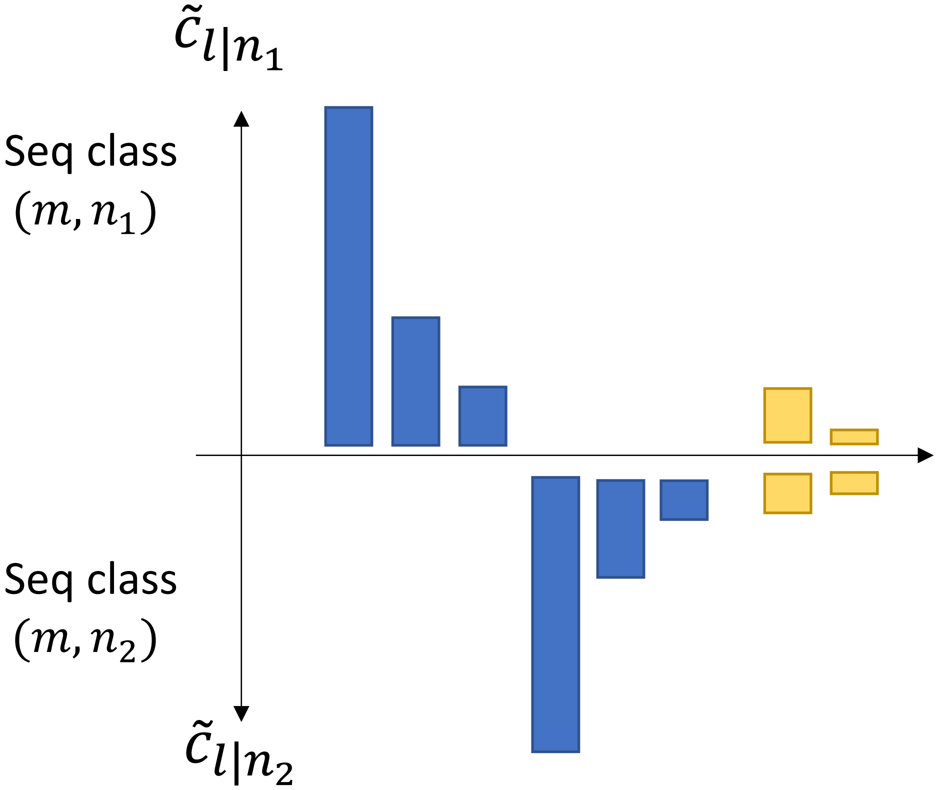
When $t \geq t_0 = O\left(\frac{2K\ln M}{\eta_Y}\right)$, $B_n(t) = O(\ln\ln t)$

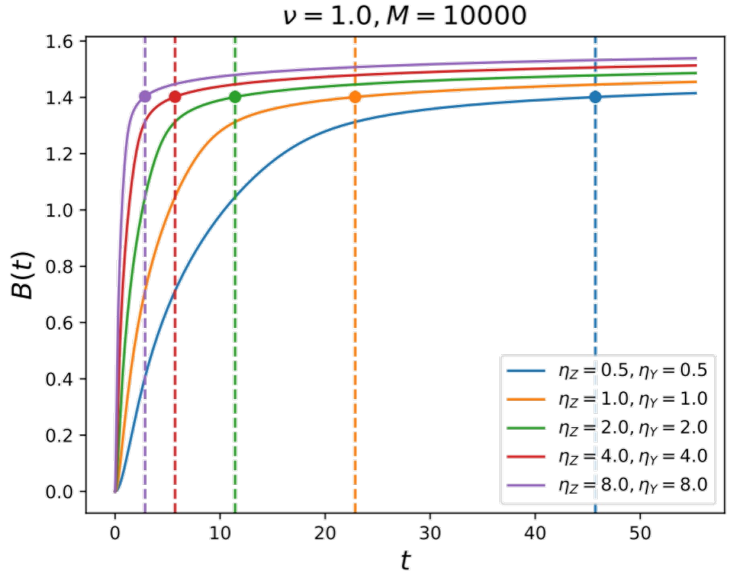
(1) η_Z and η_Y are large, $B_n(t)$ is large and attention is sparse

(2) Fixing η_Z, large η_Y leads to slightly small $B_n(t)$ and denser attention

Overall Picture of the Training Dynamics

Attention frozen





Larger learning rate η_z leads to faster phase transition

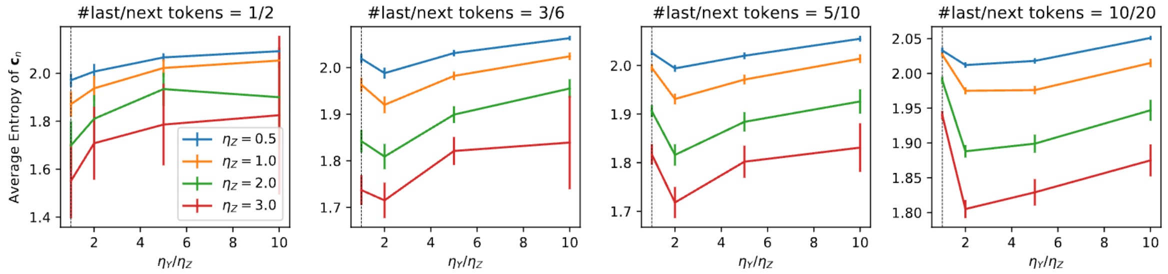
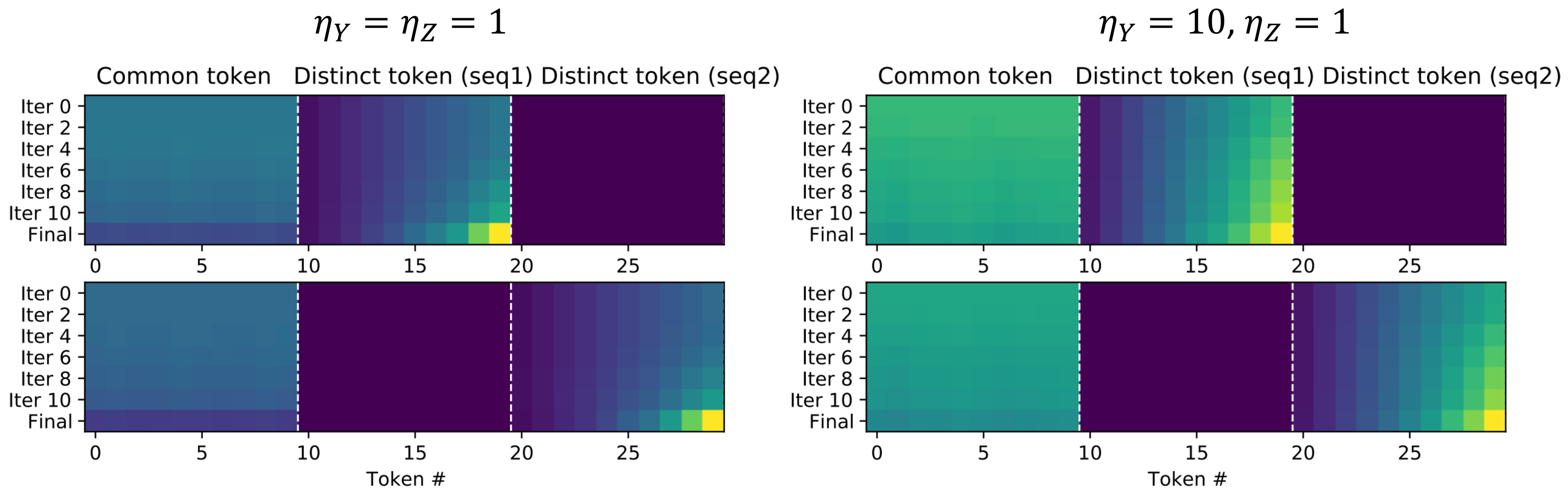


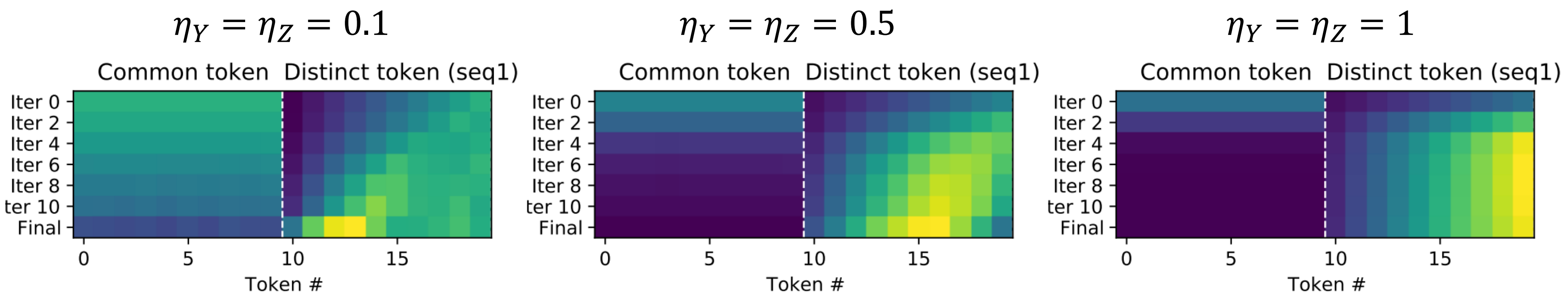
Figure 6: Average entropy of $\boldsymbol{c}_n$ (Eqn. 5) on distinct tokens versus learning rate ratio η_Y/η_Z with more last tokens M/next tokens K. We report mean values over 10 seeds and standard derivation of the mean.

Visualization of $\boldsymbol{c_n}$

SGD dynamics



Adam dynamics



Simple Real-world Experiments

WikiText2 (original parameterization)

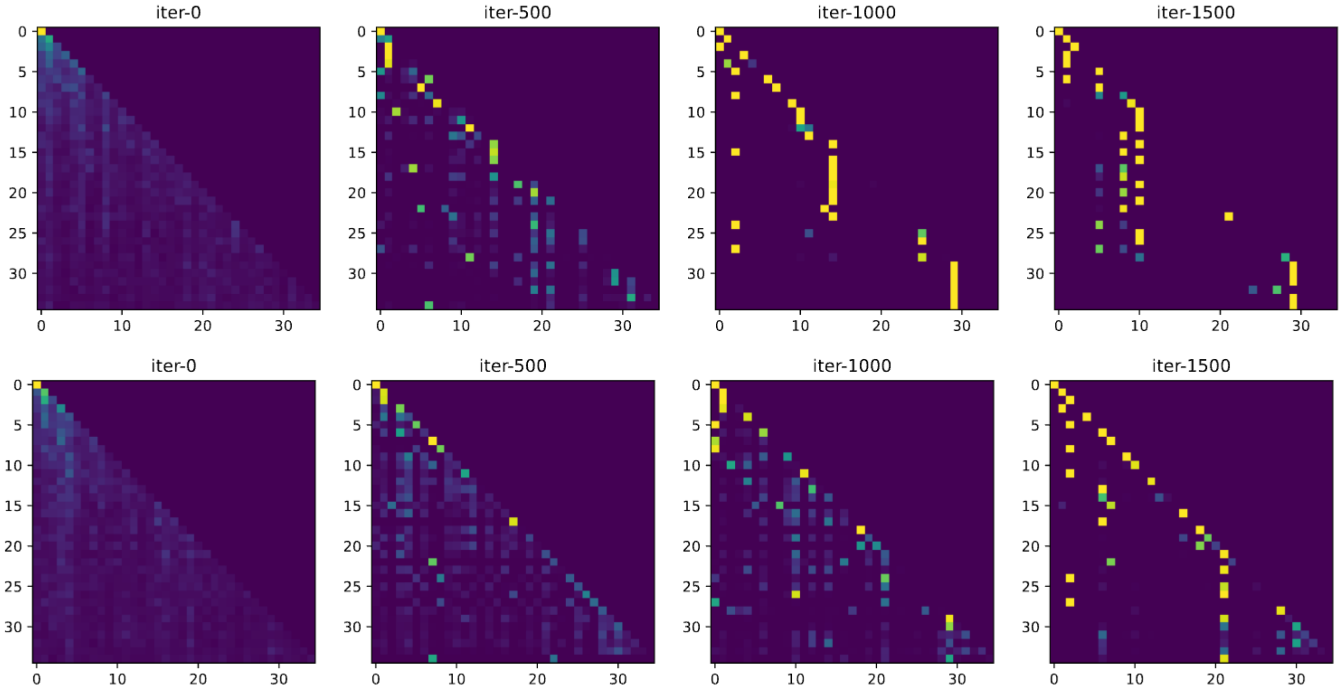


Figure 7: Attention patterns in the lowest self-attention layer for 1-layer (top) and 3-layer (bottom) Transformer trained on WikiText2 using SGD (learning rate is 5). Attention becomes sparse over training.

Overall strategy of the theoretical analysis

- The power of infinite sequence length $T \to +\infty$

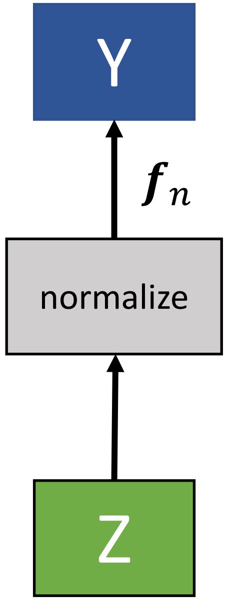
Lemma 2. *Given the event* $\{x_T = m, x_{T+1} = n\}$, *when* $T \to +\infty$, *we have*

$$X^\top \boldsymbol{b}_T \to \boldsymbol{c}_{m,n}, \qquad X^\top \mathrm{diag}(\boldsymbol{b}_T) X \to \mathrm{diag}(\boldsymbol{c}_{m,n})$$

where $\boldsymbol{c}_{m,n} = [c_{1|m,n}, c_{2|m,n}, \ldots, c_{M|m,n}]^\top \in \mathbb{R}^M$. *Note that* $\boldsymbol{c}_{m,n}^\top \mathbf{1} = 1$.

Here $$c_{l|m,n} := \frac{T\mathbb{P}(l|m,n)\exp(z_{ml})}{\sum_{l'} T\mathbb{P}(l'|m,n)\exp(z_{ml'})} = \frac{\mathbb{P}(l|m,n)\exp(z_{ml})}{\sum_{l'} \mathbb{P}(l'|m,n)\exp(z_{ml'})} =: \frac{\tilde{c}_{l|m,n}}{\sum_{l'} \tilde{c}_{l'|m,n}}$$

Define $\boldsymbol{f}_n := \boldsymbol{f}_{m,n} := \boldsymbol{c}_{m,n} / \|\boldsymbol{c}_{m,n}\|_2$ a ℓ_2-normalized version of $\boldsymbol{c}_{m,n}$.



Overall strategy of the theoretical analysis

- Since $\eta_Y \gg \eta_Z$, we analyze the dynamics of decoder Y first, treating the output of Z as constant.

$$\dot{Y} = \eta_Y \boldsymbol{f}_n (\boldsymbol{e}_n - \boldsymbol{\alpha}_n)^\top, \quad \boldsymbol{\alpha}_n = \frac{\exp(Y^\top \boldsymbol{f}_n)}{\mathbf{1}^\top \exp(Y^\top \boldsymbol{f}_n)}$$

- The analysis gives backpropagated gradient:

Theorem 1. *If Assumption 2 holds, the initial condition* $Y(0) = 0$, $M \gg 100$, η_Y *satisfies* $M^{-0.99} \ll \eta_Y < 1$, *and each sequence class appears uniformly during training, then after* $t \gg K^2$ *steps of batch size* 1 *update, given event* $x_{T+1}[i] = n$, *the backpropagated gradient* $\boldsymbol{g}[i] := Y(\boldsymbol{x}_{T+1}[i] - \boldsymbol{\alpha}[i])$ *takes the following form:*

$$\boldsymbol{g}[i] = \gamma \left(\iota_n \boldsymbol{f}_n - \sum_{n' \neq n} \beta_{nn'} \boldsymbol{f}_{n'} \right) \tag{9}$$

Overall strategy of the theoretical analysis

- Given the backpropagated gradient, we can analyze the behavior of the self-attention layer.

Theorem 2 (Fates of contextual tokens)**.** *Let G_{CT} be the set of common tokens (CT), and $G_{DT}(n)$ be the set of distinct tokens (DT) that belong to next token n. Then if Assumption 2 holds, under the self-attention dynamics (Eqn. 10), we have:*

- ***(a)** for any distinct token $l \in G_{DT}(n)$, $\dot{z}_{ml} > 0$ where $m = \psi(n)$;*
- ***(b)** if $|G_{CT}| = 1$ and at least one next token $n \in \psi^{-1}(m)$ has at least one distinct token, then for the single common token $l \in G_{CT}$, $\dot{z}_{ml} < 0$.*

Conclusions of Scan&Snap

- Take home message
  - Dynamics of self-attention leads to *contextual sparsity*
  - Key tokens that do not co-occur a lot with the query token are suppressed.
- Application
  - Predicting Contextual Sparsity for fast LLM inference
    - **Deja Vu: Contextual Sparsity for Efficient LLMs at Inference Time (ICML'23)**
- A lot of mysteries remain.
  - Why such sparsity is important for learning?
  - How to add embedding back?
  - What's the role played by MLPs and how MLPs interact with Self-Attn?
    - **JoMA: Demystifying Multilayer Transformers via JOint Dynamics of MLP and Attention (arXiv'23)**

Thanks!