Reasoning by Superposition:

A Theoretical Perspective on Chain of Continuous Thought

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LLMs on reasoning tasks using CoT

- LLMs are powerful in many reasoning tasks, especially with chain-of-thought (CoT)

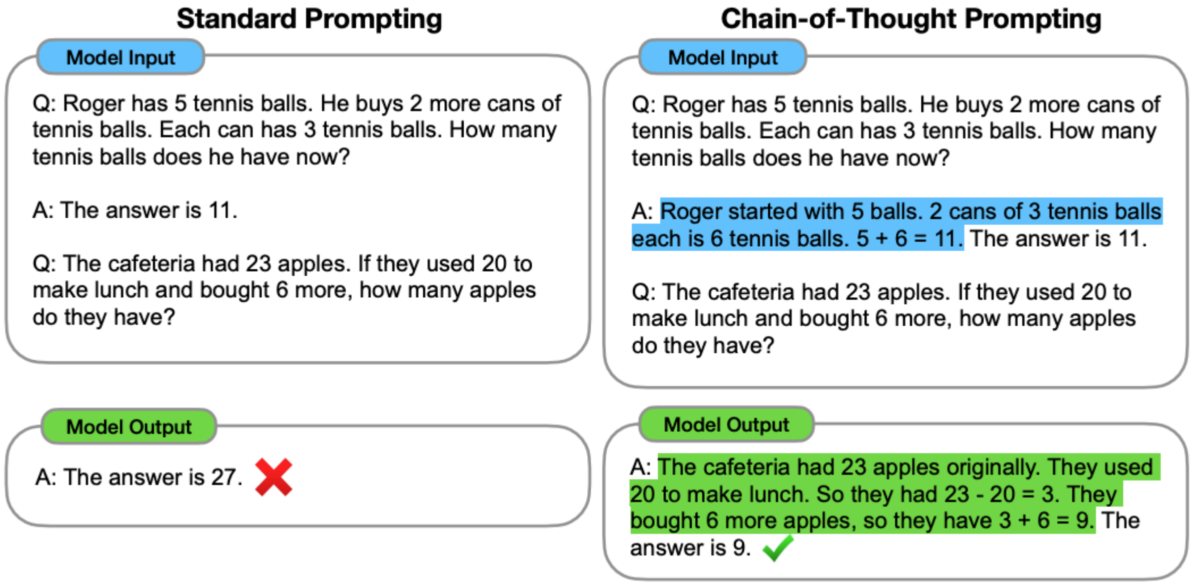


Figure credit to [1]

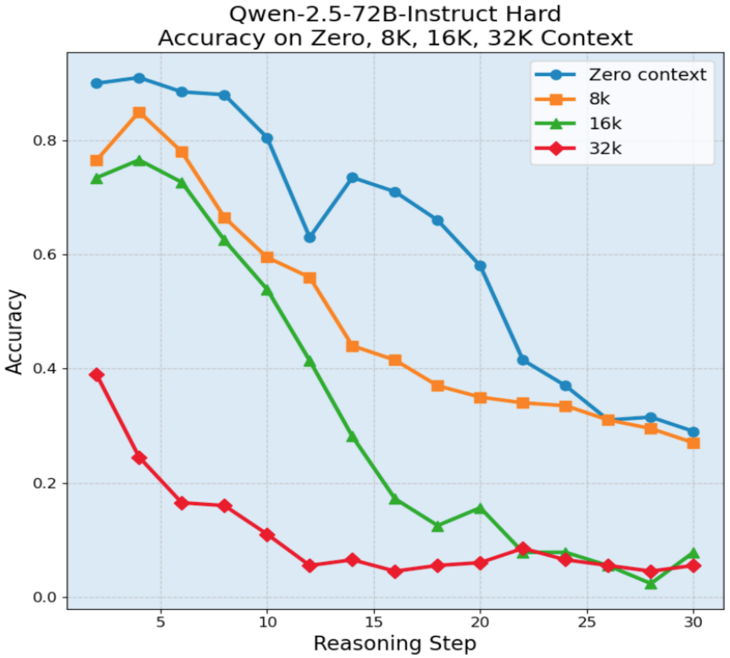


Figure credit to [2]

- LLMs still struggle with more complex reasoning tasks (e.g., longer reasoning steps)
- How to expand existing CoT methods to solve more complex problems?

[1] Wei, Jason, Xuezhi Wang, Dale Schuurmans, Maarten Bosma, Fei Xia, Ed Chi, Quoc V. Le, and Denny Zhou. "Chain-of-thought prompting elicits reasoning in large language models." NeurIPS'22
[2] Zhou, Yang, Hongyi Liu, Zhuoming Chen, Yuandong Tian, and Beidi Chen. "GSM-Infinite: How Do Your LLMs Behave over Infinitely Increasing Context Length and Reasoning Complexity?." *ICML'25*

Chain of continuous thought

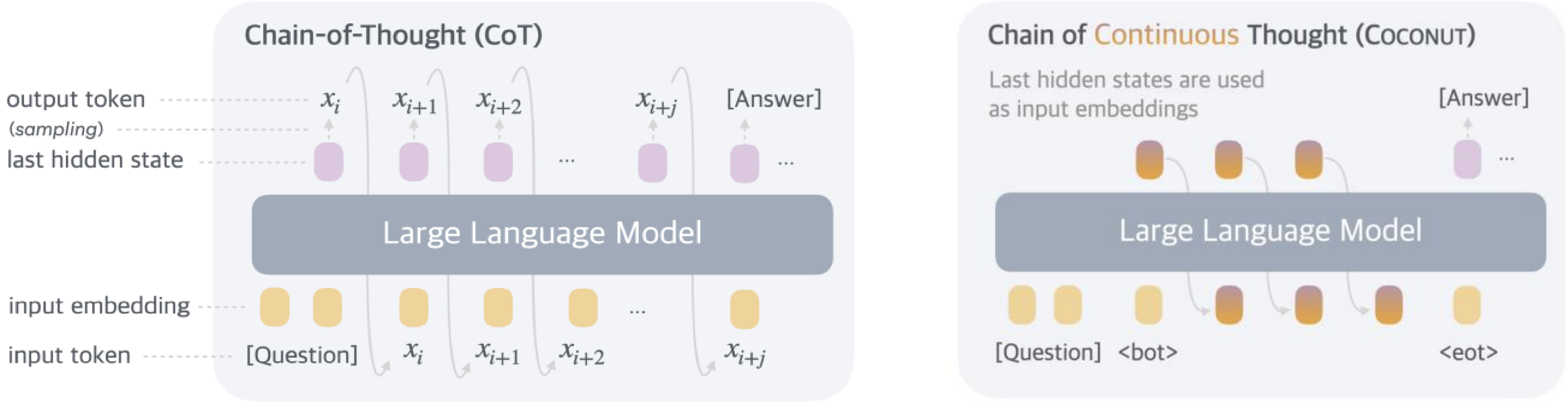


Figure credit to [1]

- Continuous CoT: directly uses the hidden state as the next input
- Outperforms discrete CoTs in various reasoning tasks
  - Especially problems with high branching factors/requires searching
- Lacks theoretical understanding of its power and mechanism

[1] Hao, Shibo, Sainbayar Sukhbaatar, DiJia Su, Xian Li, Zhiting Hu, Jason Weston, and Yuandong Tian. "Training large language models to reason in a continuous latent space." *COLM'25*

Main results

- *Construct* a 2-layer transformer with Continuous CoT that *solves* directed graph reachability using $O(n)$ steps (n: # of vertices)
  - The best known result for constant-depth transformers with discrete CoT requires $O(n^2)$ steps[1]

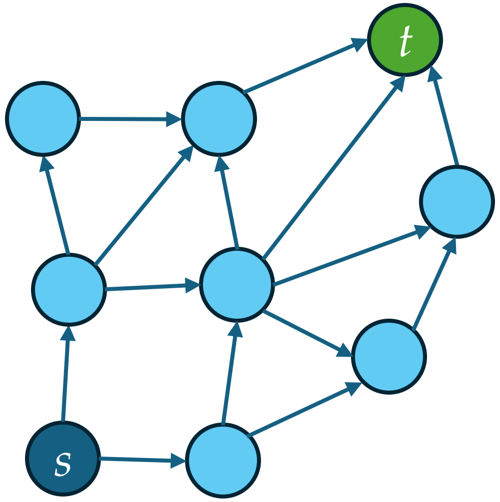
- **Insights:** Continuous thoughts maintain a "superposition" of explored vertices, performing a parallel BFS

- Empirical study is aligned with theoretical construction
  - Superposition representation **emerges** during training (no supervision)

[1] Merrill, William, and Ashish Sabharwal. "The expressive power of transformers with chain of thought." *arXiv preprint arXiv:2310.07923* (2023).

Problem Definition: Graph reachability

- Given a directed graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$, decide whether a node $\boldsymbol{s}$ can reach $\boldsymbol{t}$
  - Many real-world reasoning problem can be abstracted as a graph (e.g., knowledge graph)
  - Many theoretical problems can be reduced to it (e.g., Turing machine halting problem)



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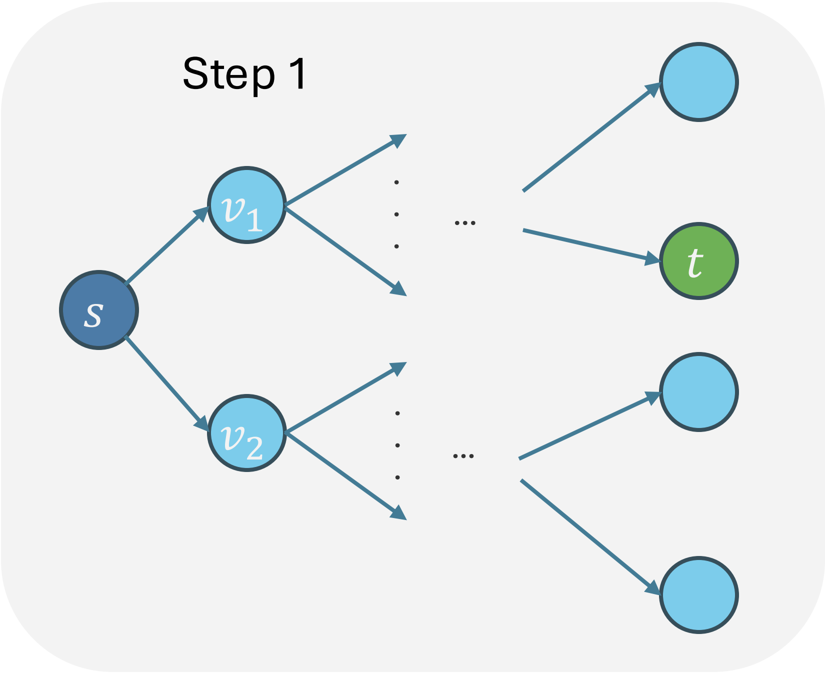

Search process

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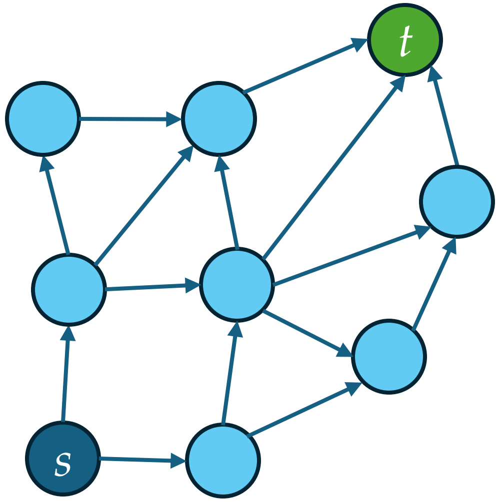

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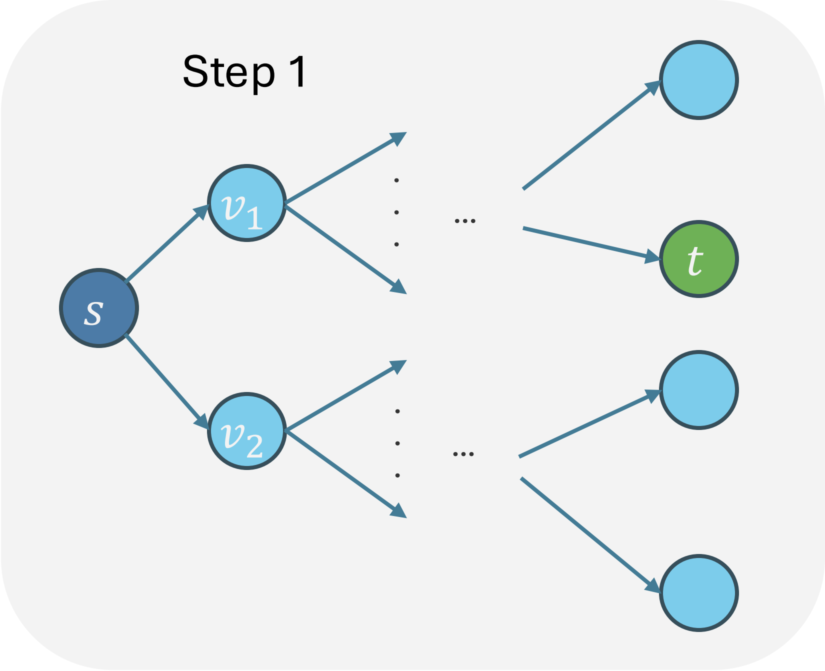

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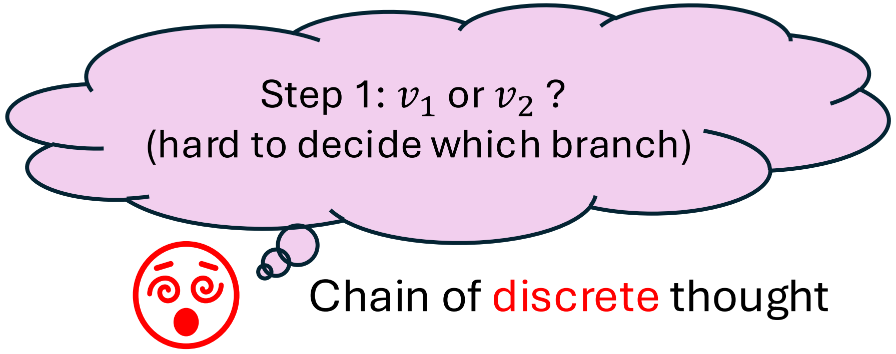

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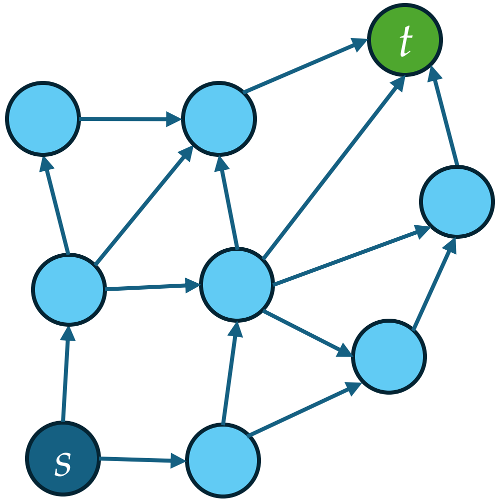

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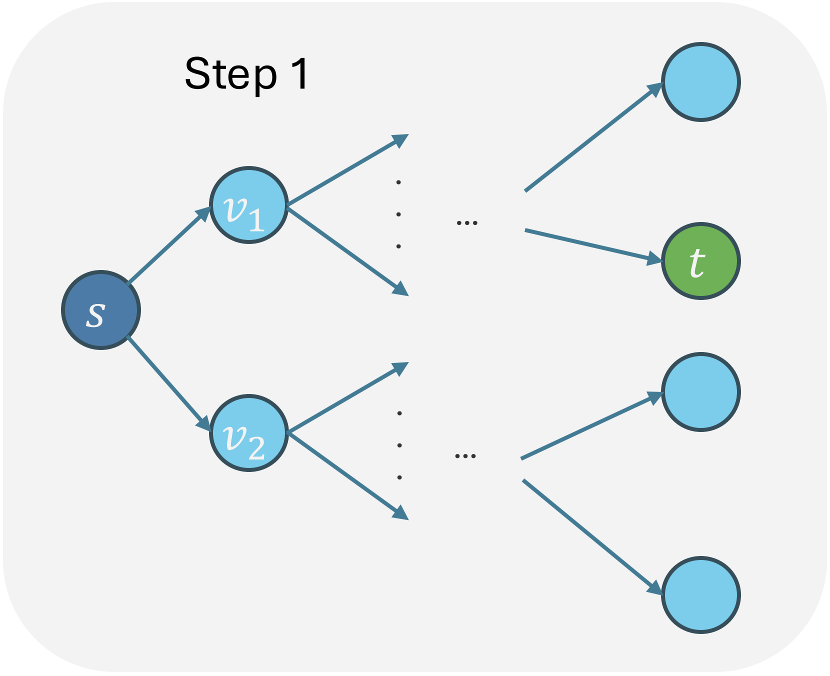

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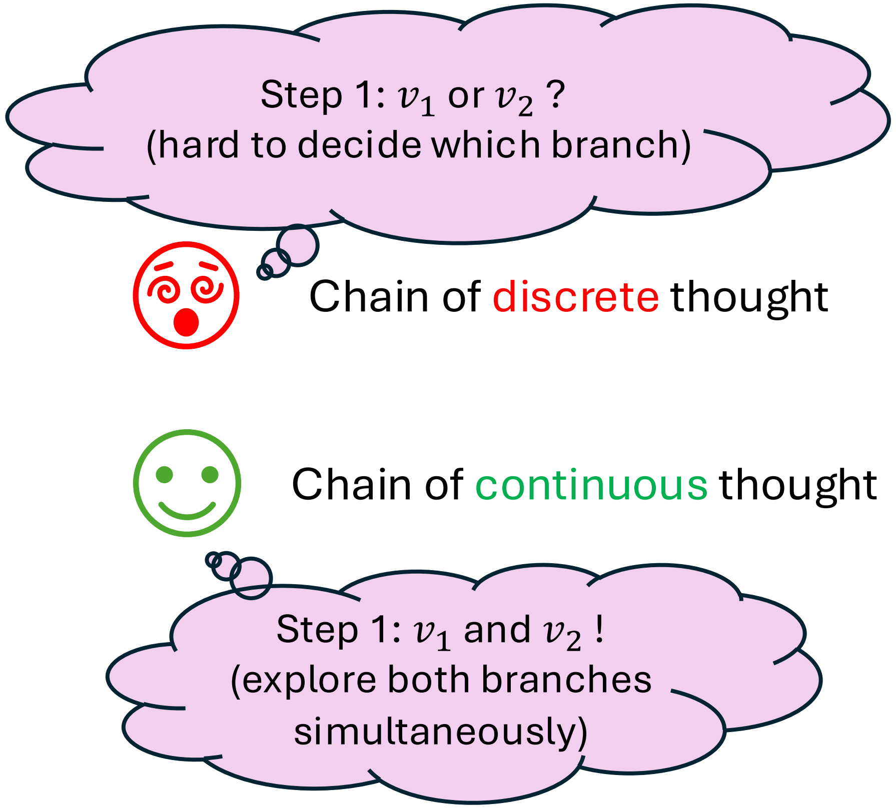
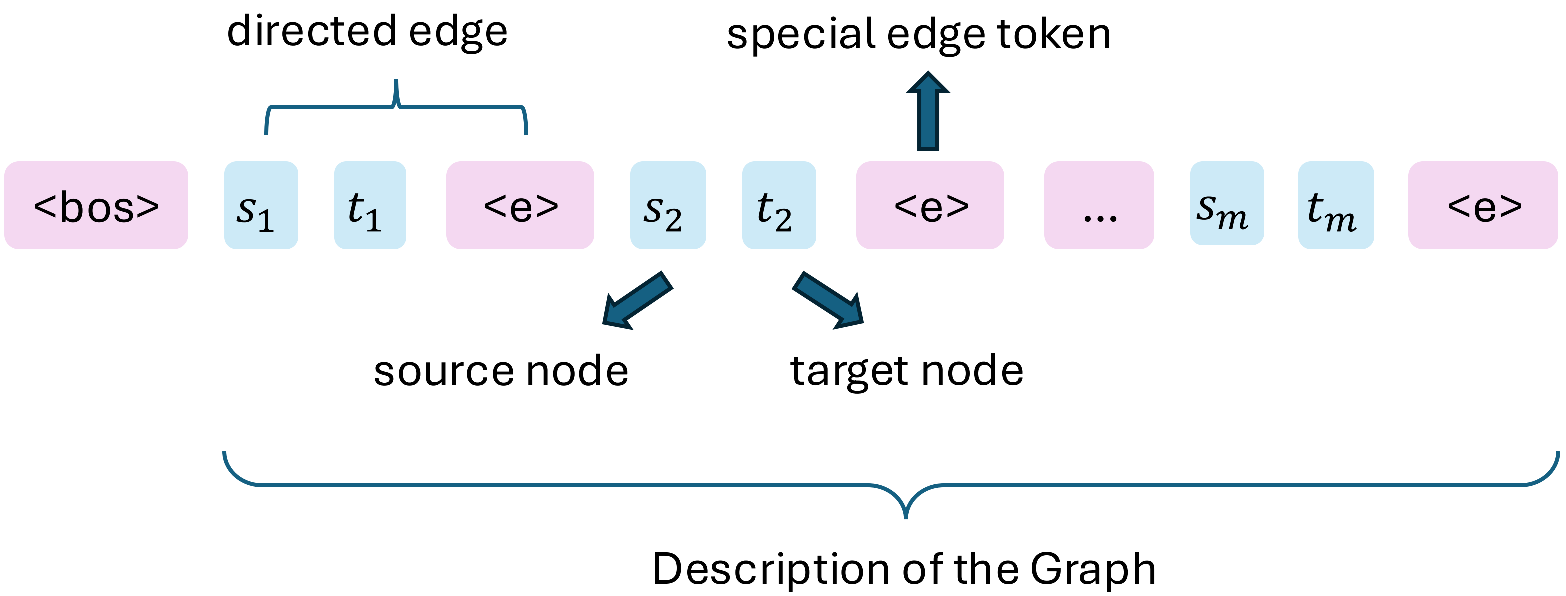


Prompt format

Given two candidate destination nodes, decide which one can be reached



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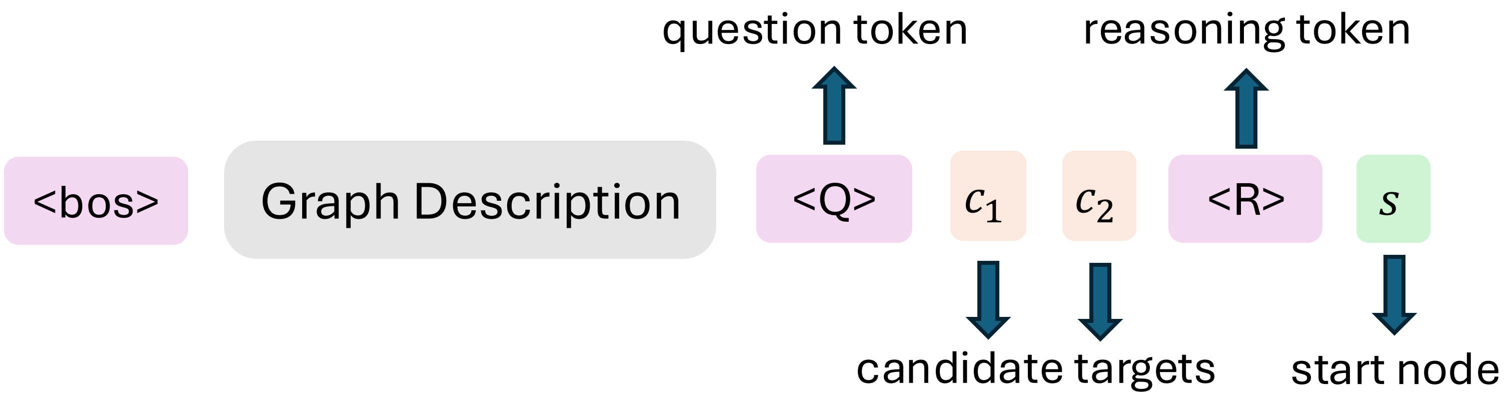

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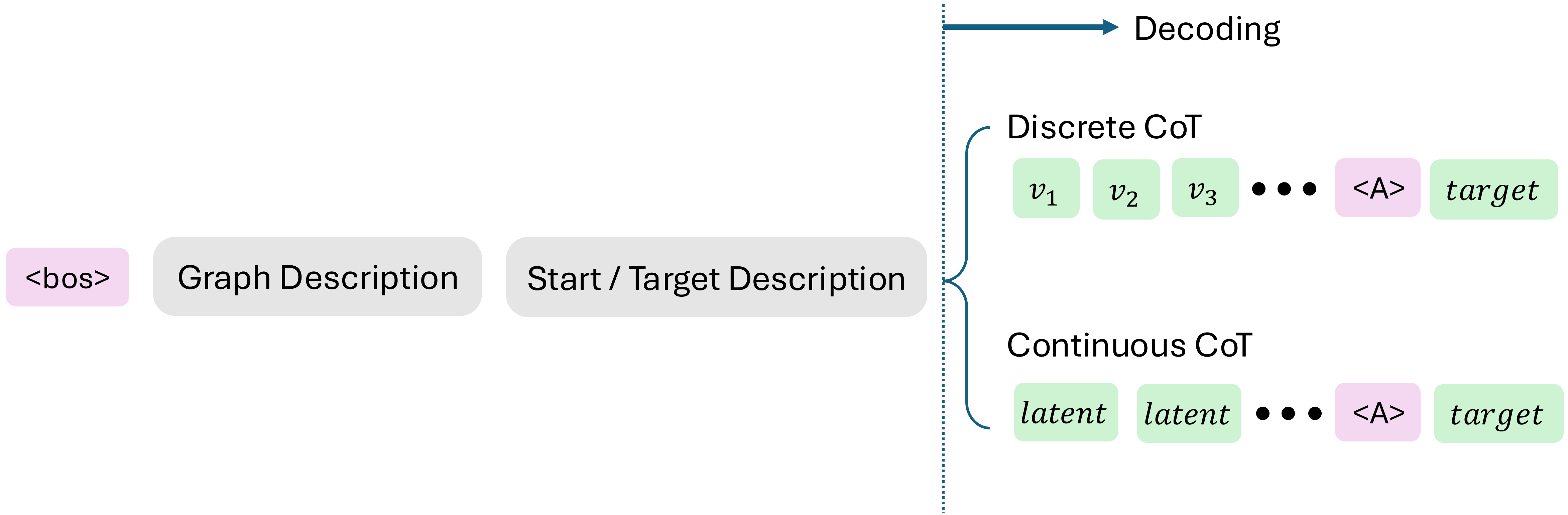


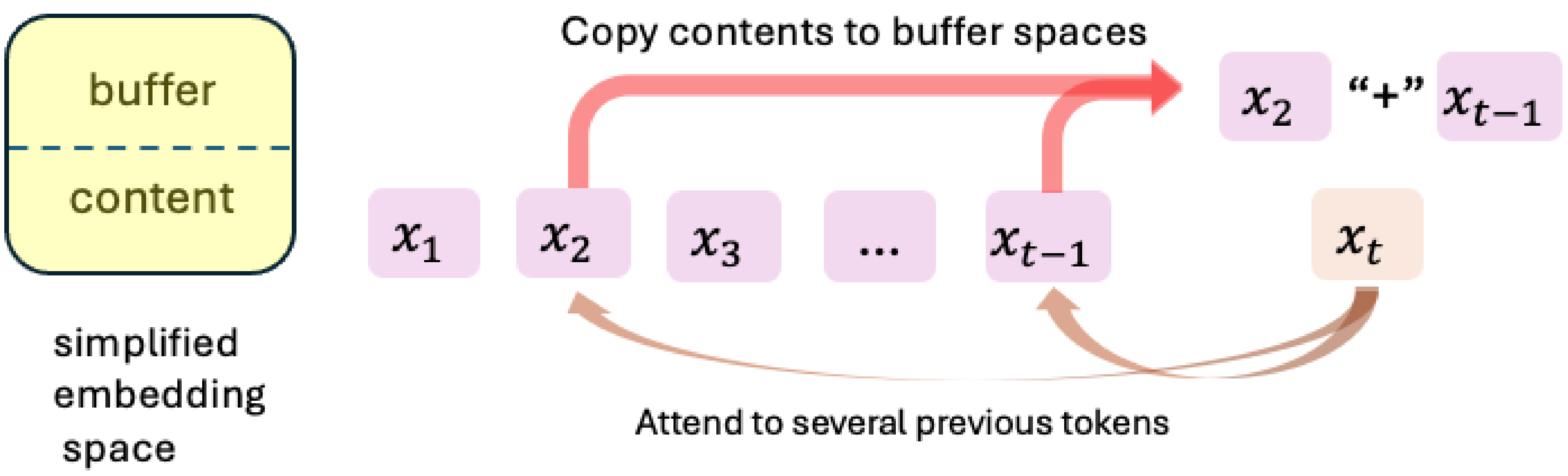
Main theorem

Theorem (informal)

For n-vertex directed graphs, a **2-layer** transformer with continuous CoT can solve reachability using $O(n)$ decoding steps with $O(n)$ embedding dimensions.

Secret Sauce: Superposition of the embeddings!

Mechanism in a single Attn-MLP block



Attention as an aggregator:

- Aggregate the information along the sequence axis.
- Form a superposition of concepts.

MLP as a filter:

- Filter out the involved embedding that are not strong enough

Mechanism in a single Attn-MLP block

$$h = \sum_{v \in \mathrm{Voc}} \lambda_v \vec{u}_v$$

MLP as a filter

$$h' = W_2 \sigma(W_1 h)$$
$$= U \sigma(U^T h)$$

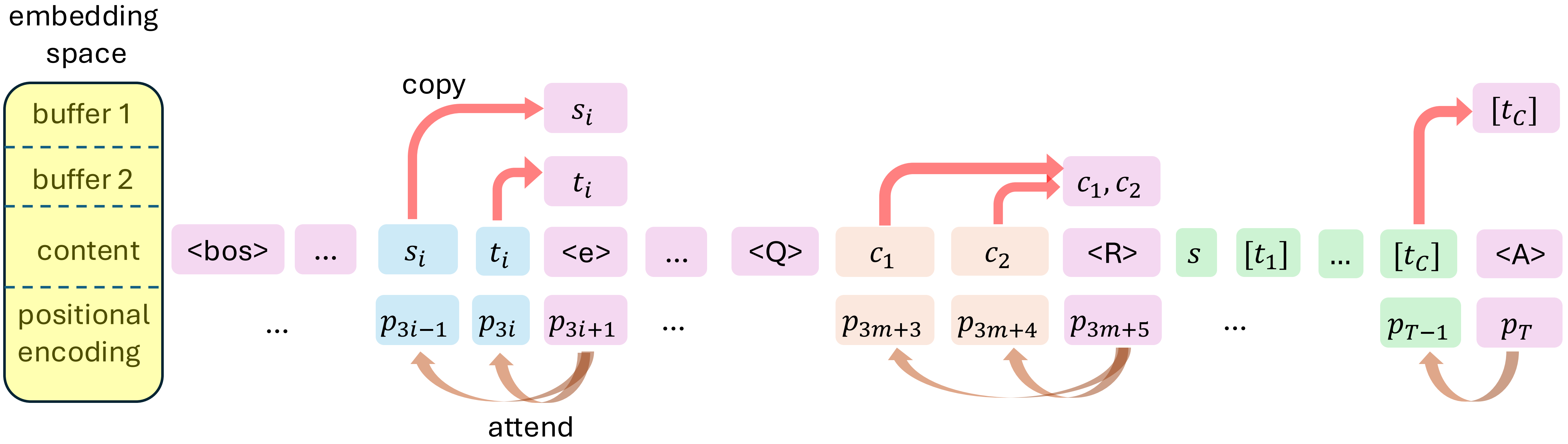
$$h' \propto \sum_{v \in \mathrm{Voc}} \mathbb{I}\{\lambda_v \geq \varepsilon\} \vec{u}_v$$

Eliminate noise

$U = [\vec{u}_1, \vec{u}_2, \ldots, \vec{u}_M]$: the embedding matrix

First-layer attention

Goal: collect all history information together into embedding space.

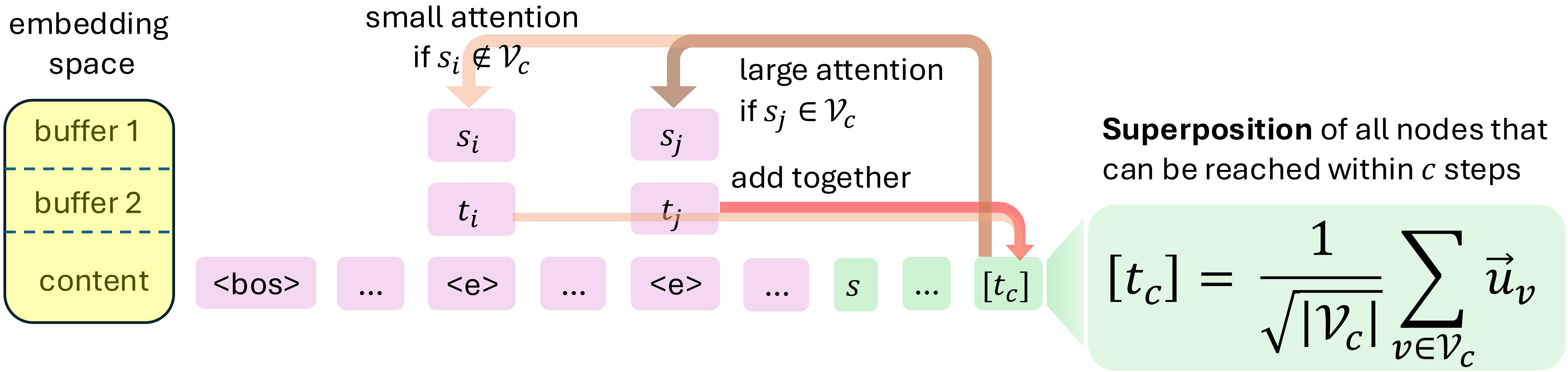


$[t_c]$ Continuous thought at step c

<A> Special answer token

FFN layers: removing low-attended embeddings

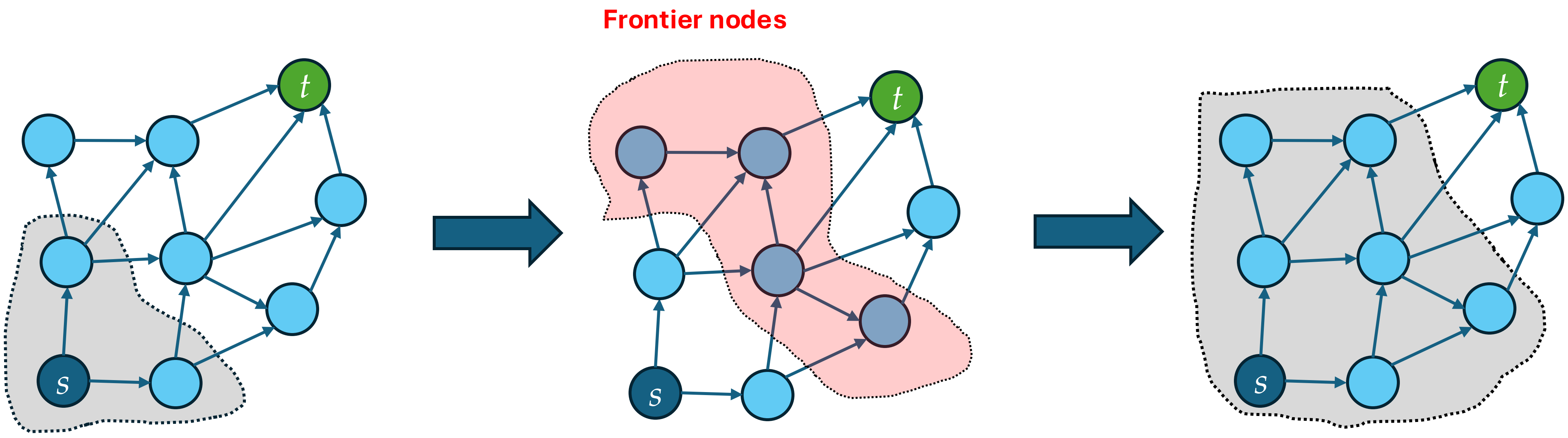
Second-layer attention



One-step expansion of $\mathcal{V}_c$

FFN layers: removing low-attended embeddings

Continuous CoT: Decoding as search



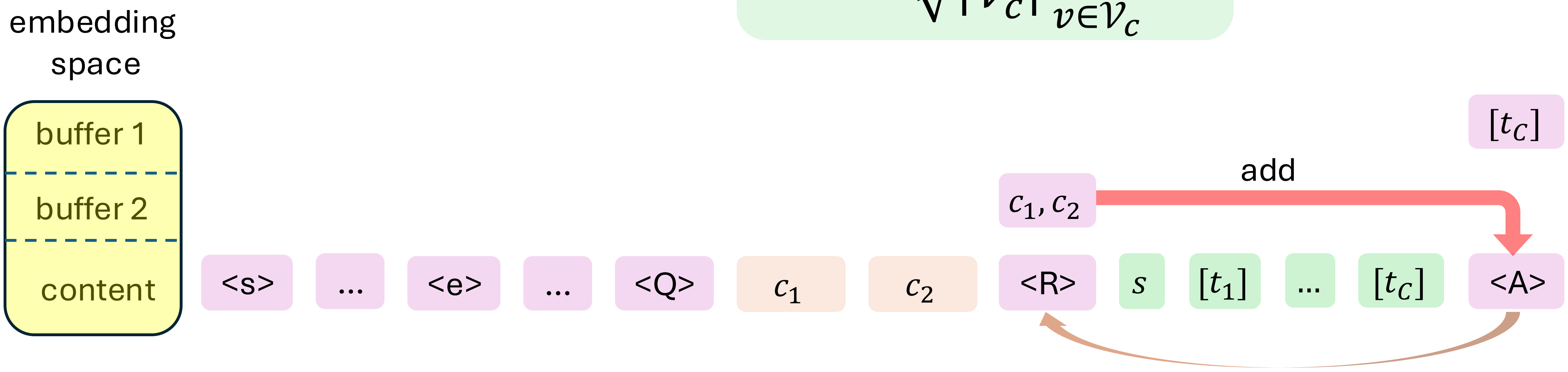
$$[t_1] = \frac{1}{\sqrt{|\mathcal{V}_1(s)|}} \sum_{v \in \mathcal{V}_1} \vec{u}_v$$

$$[t_2] = \frac{1}{\sqrt{|\mathcal{V}_2(s)|}} \sum_{v \in \mathcal{V}_2} \vec{u}_v$$

Autoregressive Decoding

$$[t_c] = \frac{1}{\sqrt{|\mathcal{V}_c|}} \sum_{v \in \mathcal{V}_c} \vec{u}_v$$

Reachable set from the starting point



"Measure" $[t_C]$ using c_1 and c_2

The target c that overlaps with **reachable set** will be picked and returned

Autoregressive Decoding

$$[t_c] = \frac{1}{\sqrt{|\mathcal{V}_c|}} \sum_{v \in \mathcal{V}_c} \vec{u}_v$$

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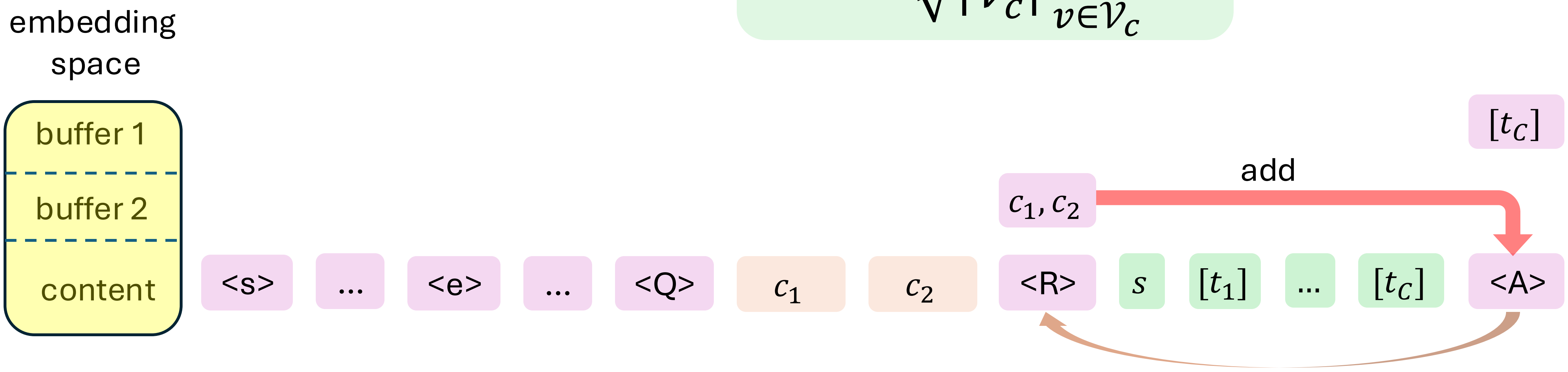

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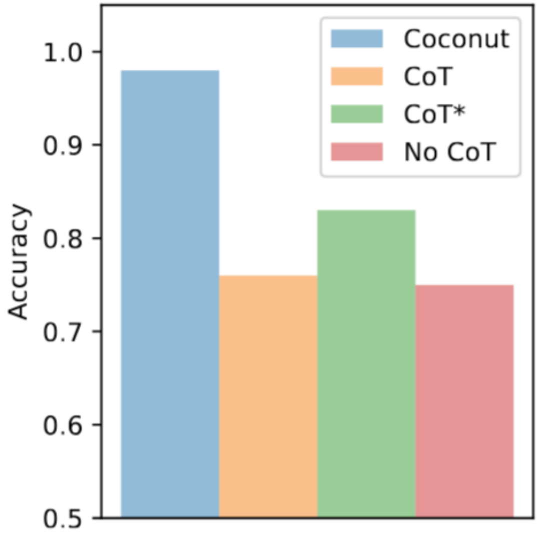
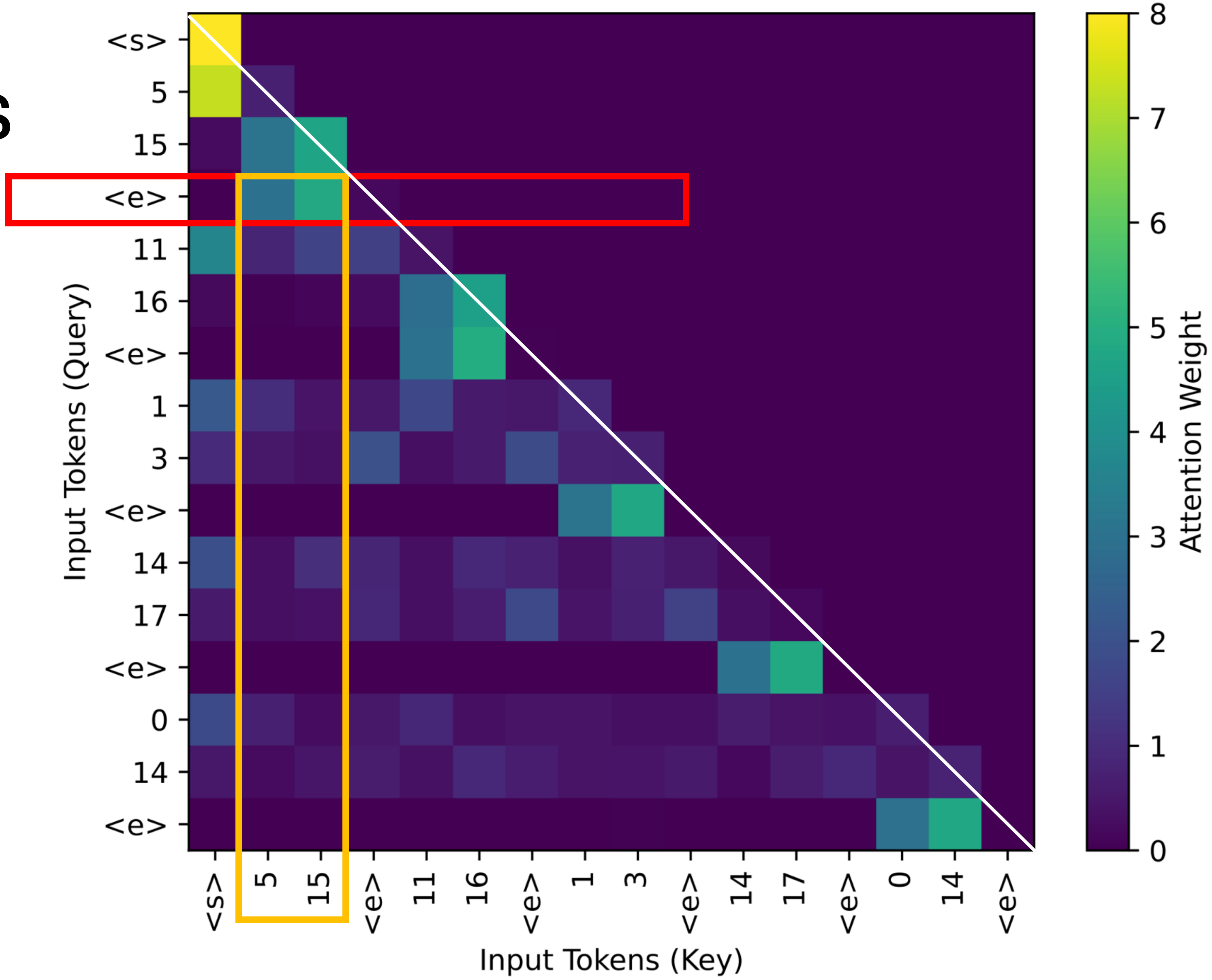
Comparison of continuous and discrete CoT

- Dataset: a subset of ProsQA[1], symbolic sequence, 3-4 steps
- Model: GPT2-style decoder
- Training: multi-stage training, stage i predicts i-th node in the optimal path using previous thoughts
- Overall results: 2-layer transformer with continuous CoT (Coconut) beats 12-layer transformer with discrete CoT (CoT*)



[1] Hao, Shibo, Sainbayar Sukhbaatar, DiJia Su, Xian Li, Zhiting Hu, Jason Weston, and Yuandong Tian. "Training large language models to reason in a continuous latent space." *arXiv preprint arXiv:2412.06769* (2024).

Layer 1
Attention Patterns



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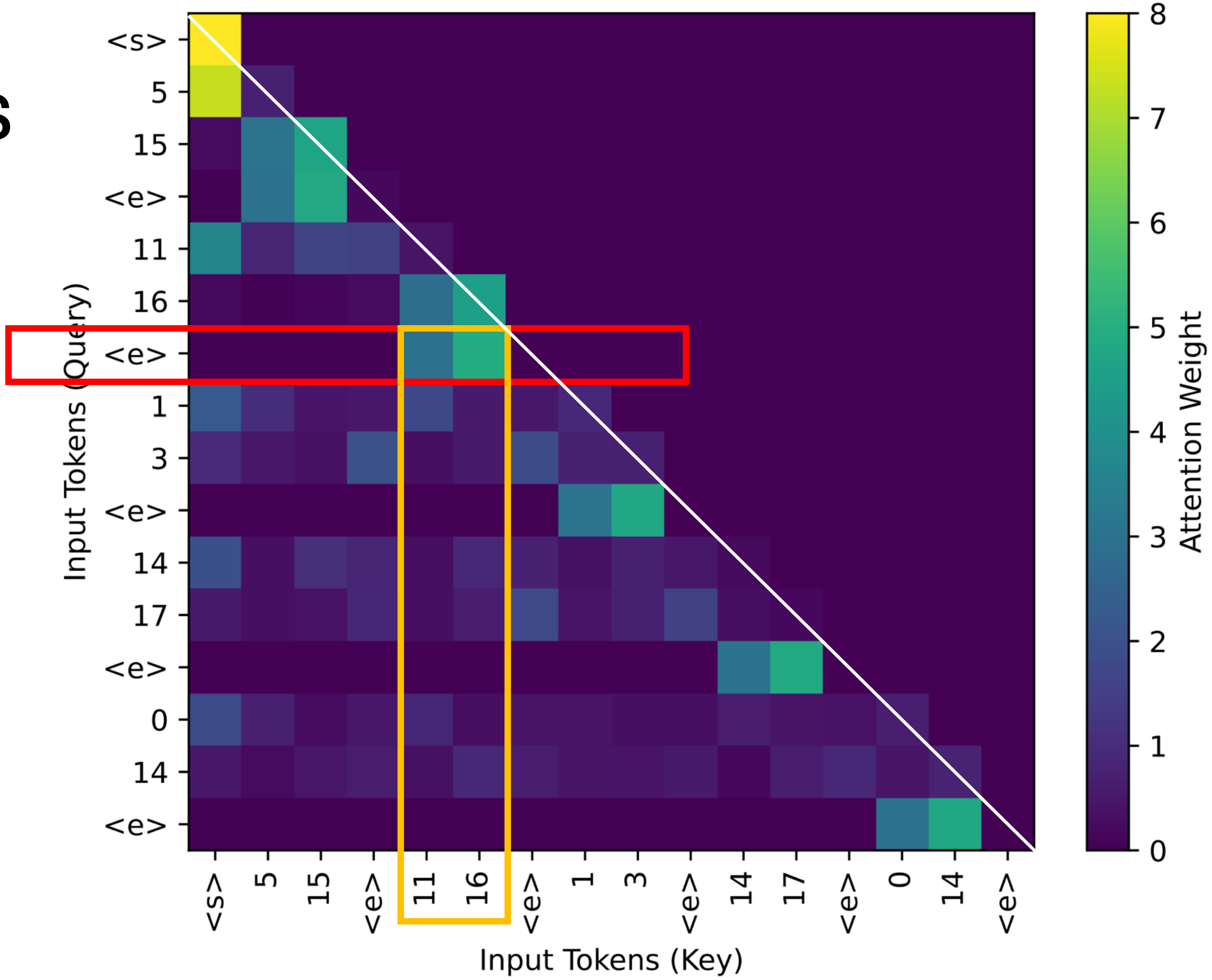

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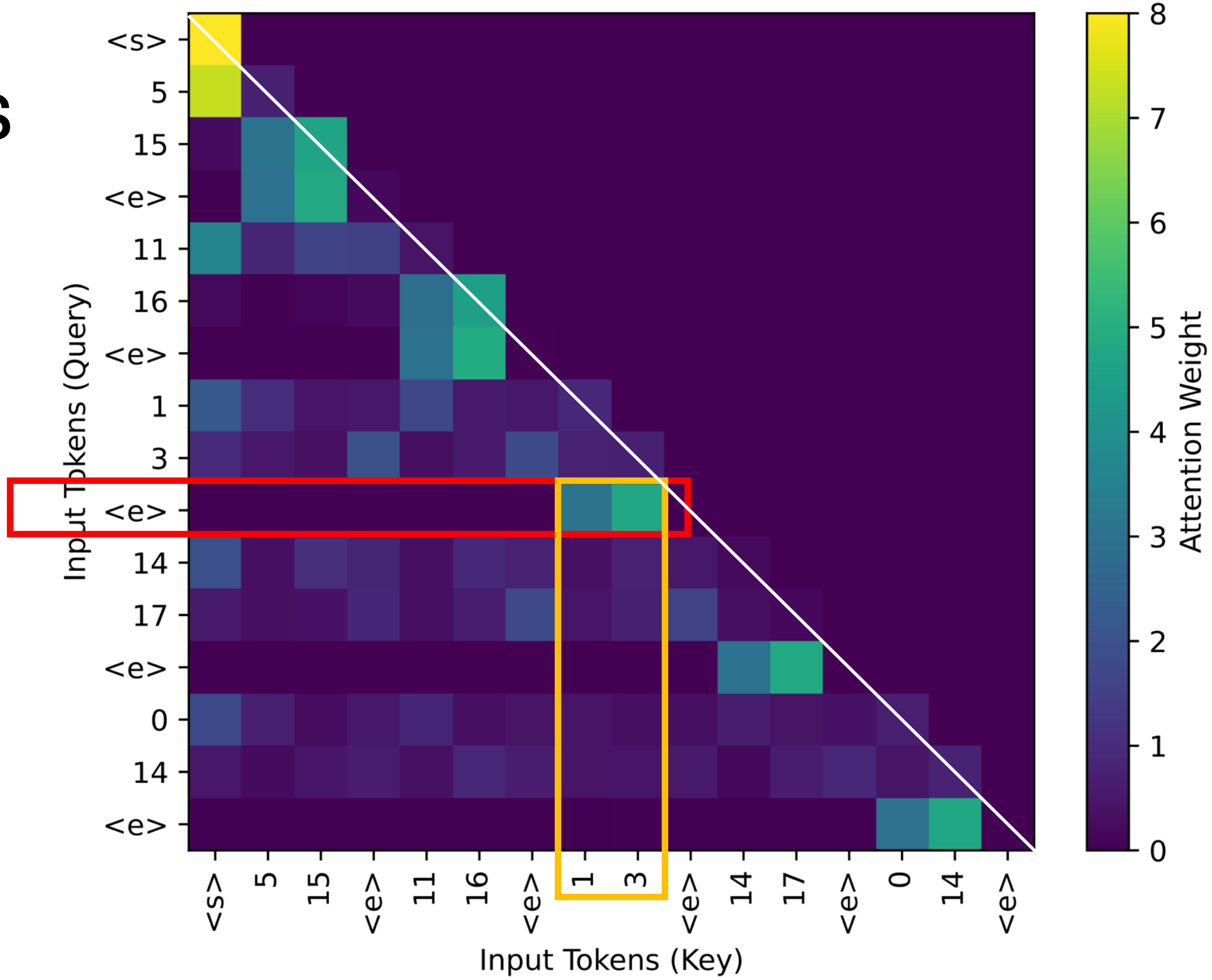
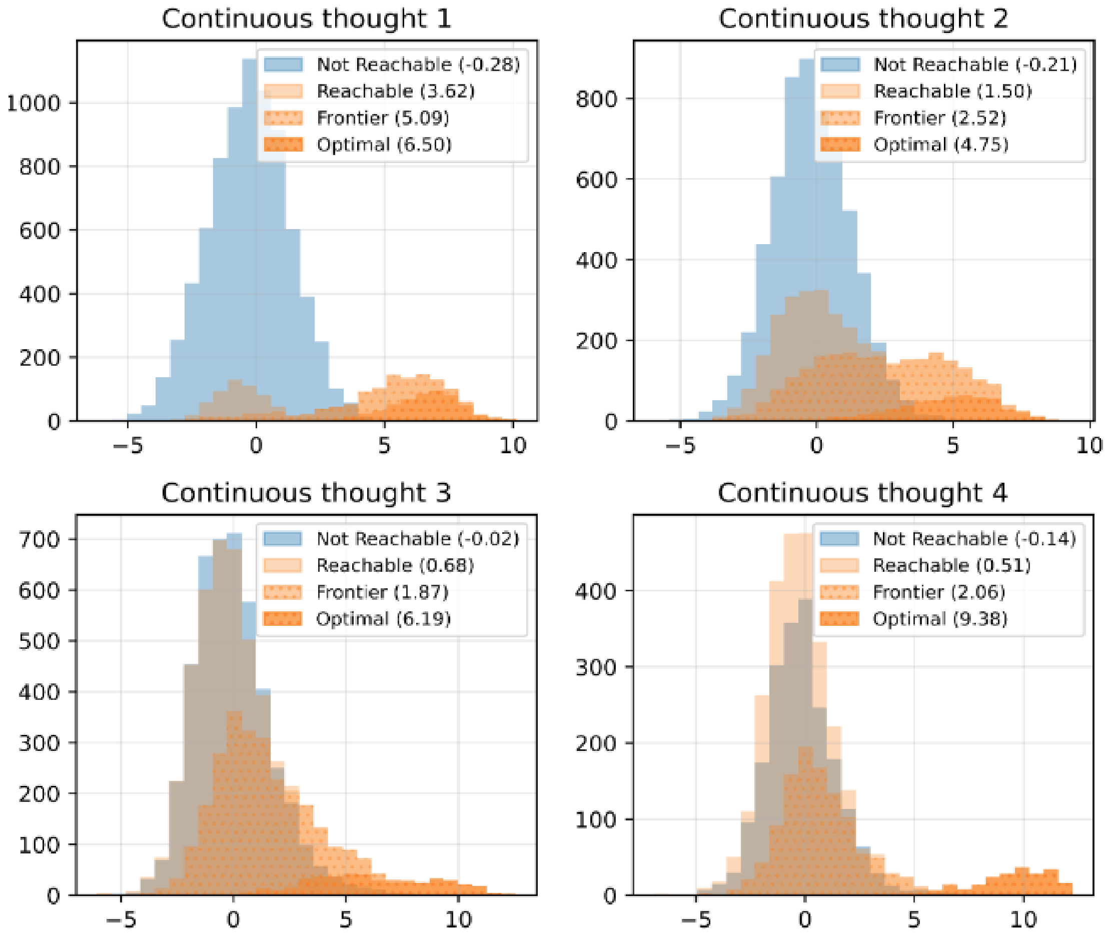


Superposition **emerges** during training

Inner products of the current thought and each node embedding

$$[t_c] = \frac{1}{\sqrt{|\mathcal{V}_c|}} \sum_{v \in \mathcal{V}_c} \vec{u}_v$$



COCONUT

Four Kinds of Nodes

- **Reachable node** (reachable from start node within i-th steps)
  - *Frontier node* (exactly i-th steps)
  - *Optimal node* (on the shortest path from the start node to the destination node)
- **Non-reachable node**

Coconut automatically **learns** to encode **frontier/optimal** nodes (**emerging!**)

Discussions

- Continuous thoughts can be powerful but hard to control
  - E.g., superposition states can be a subset of tokens (with different weights)
  - It can emerge even if the training data only contain single discrete traces
- Requires a deeper understanding if we want to use it reliably
  - Mechanism for more general tasks
  - How superposition emerges during training and how to control it

Thanks!