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Lecture 3
CME 295: Transformers & Large Language Models
Afshine Amidi & Shervine Amidi
Stanford University
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Recap of last episode...

3 categories of Transformer-based models:

Encoder-decoder	Text to text	T5, mT5, ByT5

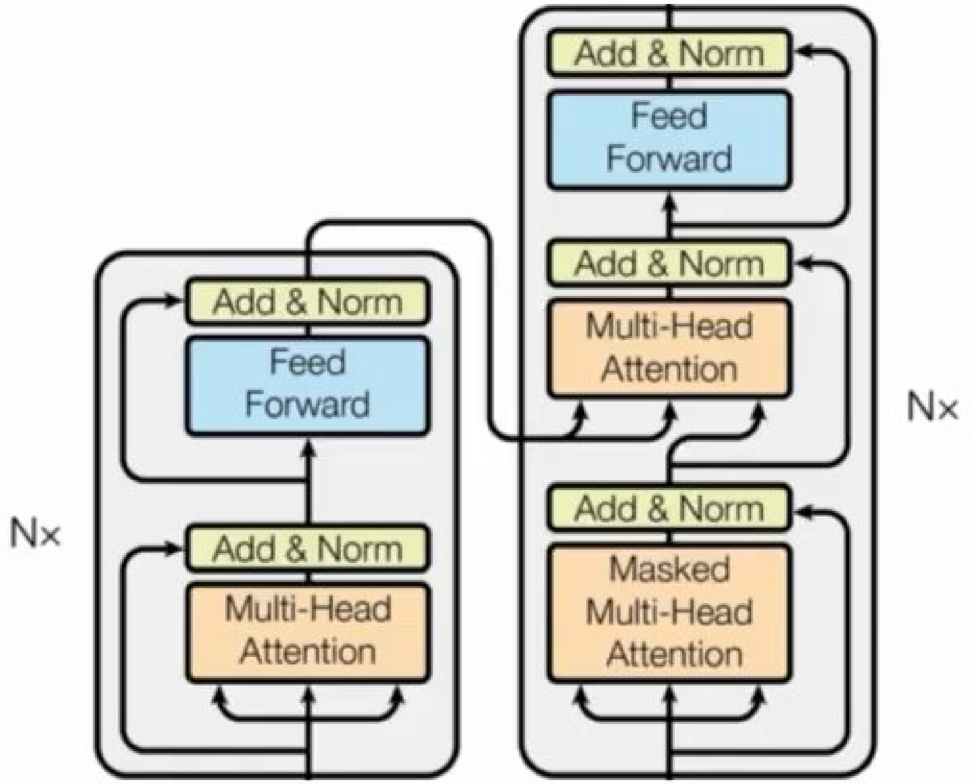

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Figure adapted from "Attention is All You Need", Vaswani et al., 2017.


Recap of last episode...
3 categories of Transformer-based models:
Encoder-only
Projection of embedding for class prediction (e.g. sentiment extraction)
BERT, DistilBERT, RoBERTa
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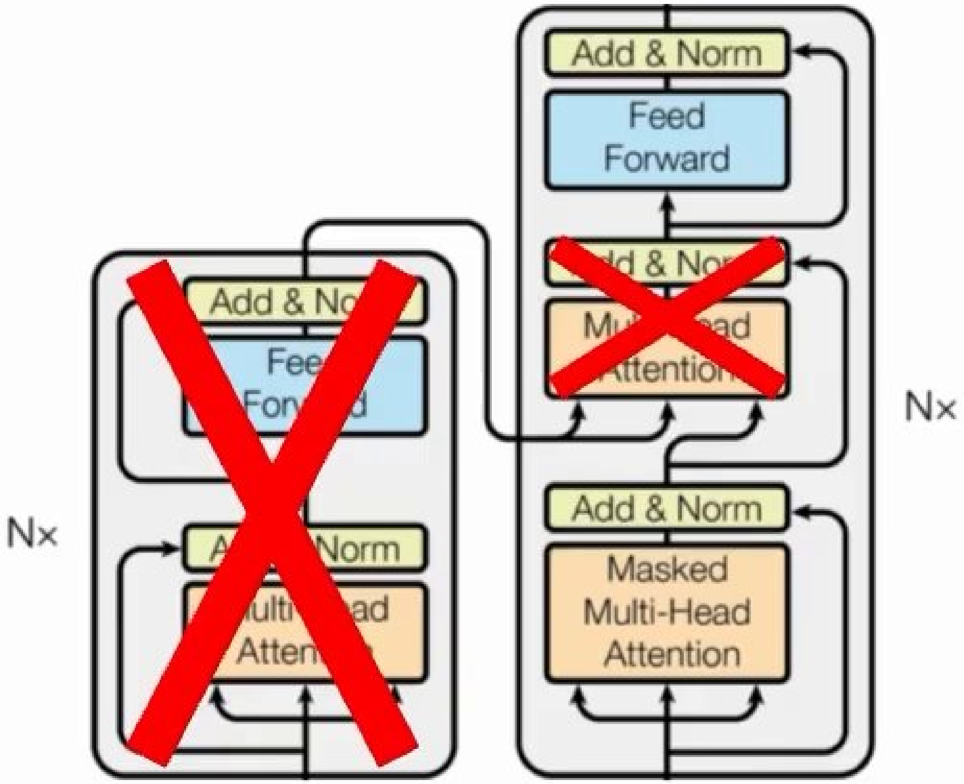
Decoder-only	Text to text	GPT series



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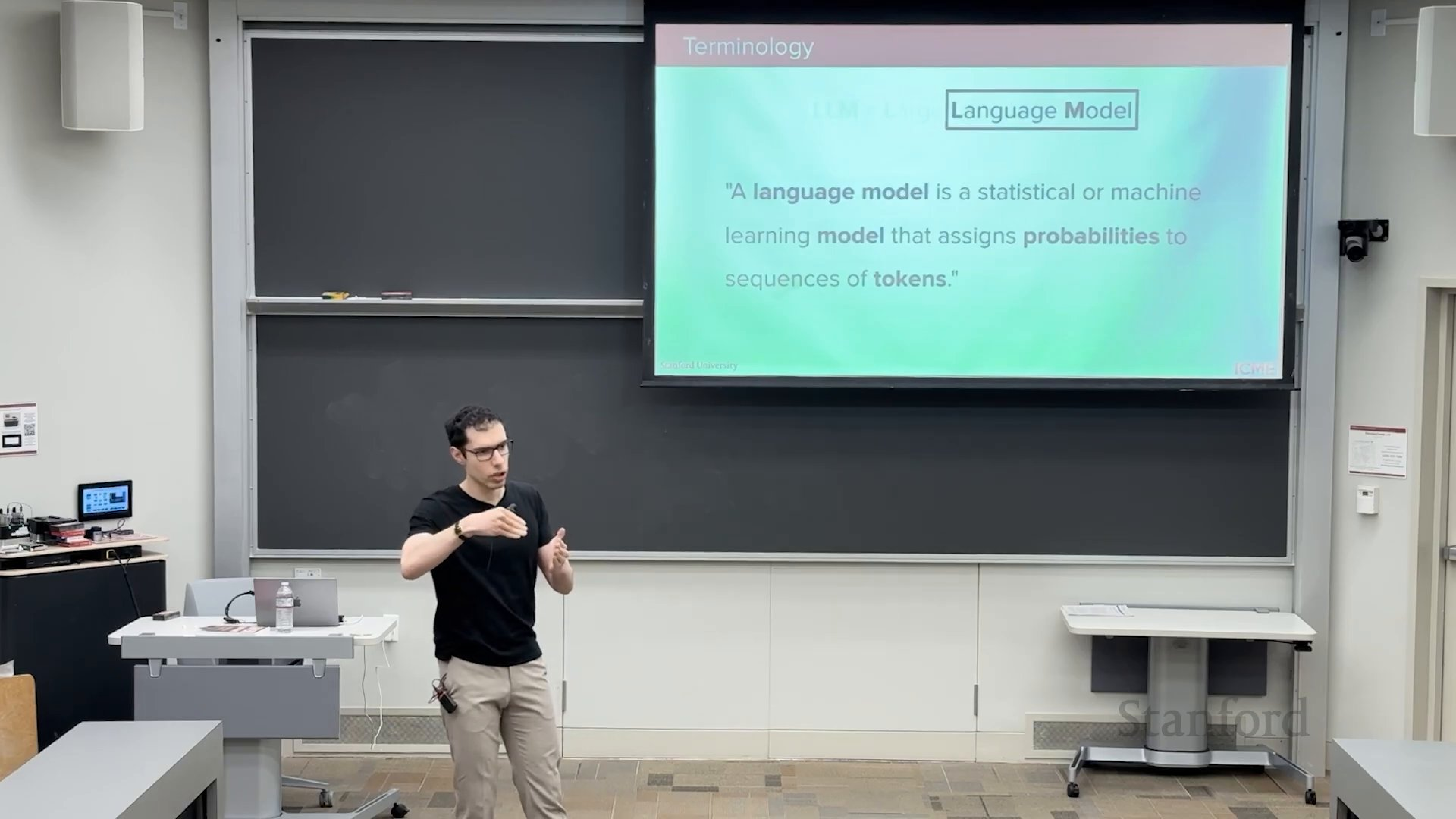
Terminology

LLM = **L**arge **L**anguage **M**odel


Terminology
Language Model
"A language model is a statistical or machine learning model that assigns probabilities to sequences of tokens."
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Terminology

LLM = $\boxed{\text{Large}}$ Language Model

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Terminology
Large
Model size: billions of parameters or more
Training data: 100s of billions of tokens or more
Compute: a lot of GPUs
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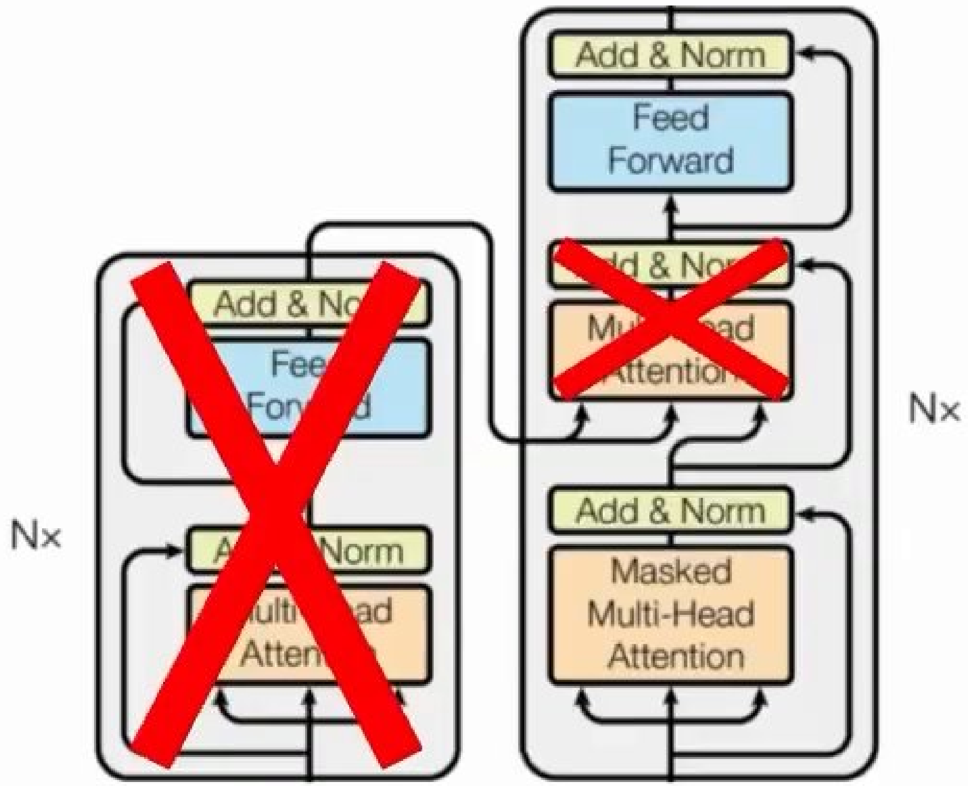
Characteristics

Decoder-only **Transformer**-based model



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Characteristics
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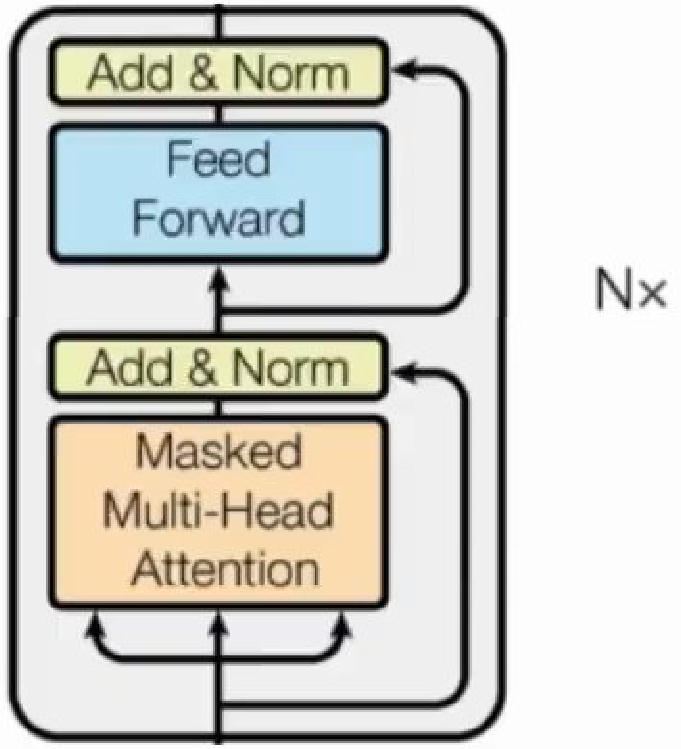

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Figure adapted from "Attention is All You Need", Vaswani et al., 2017.

Transformers & Large Language Models

LLM overview

MoE-based LLMs

Response generation

Prompting strategies

Inference optimizations

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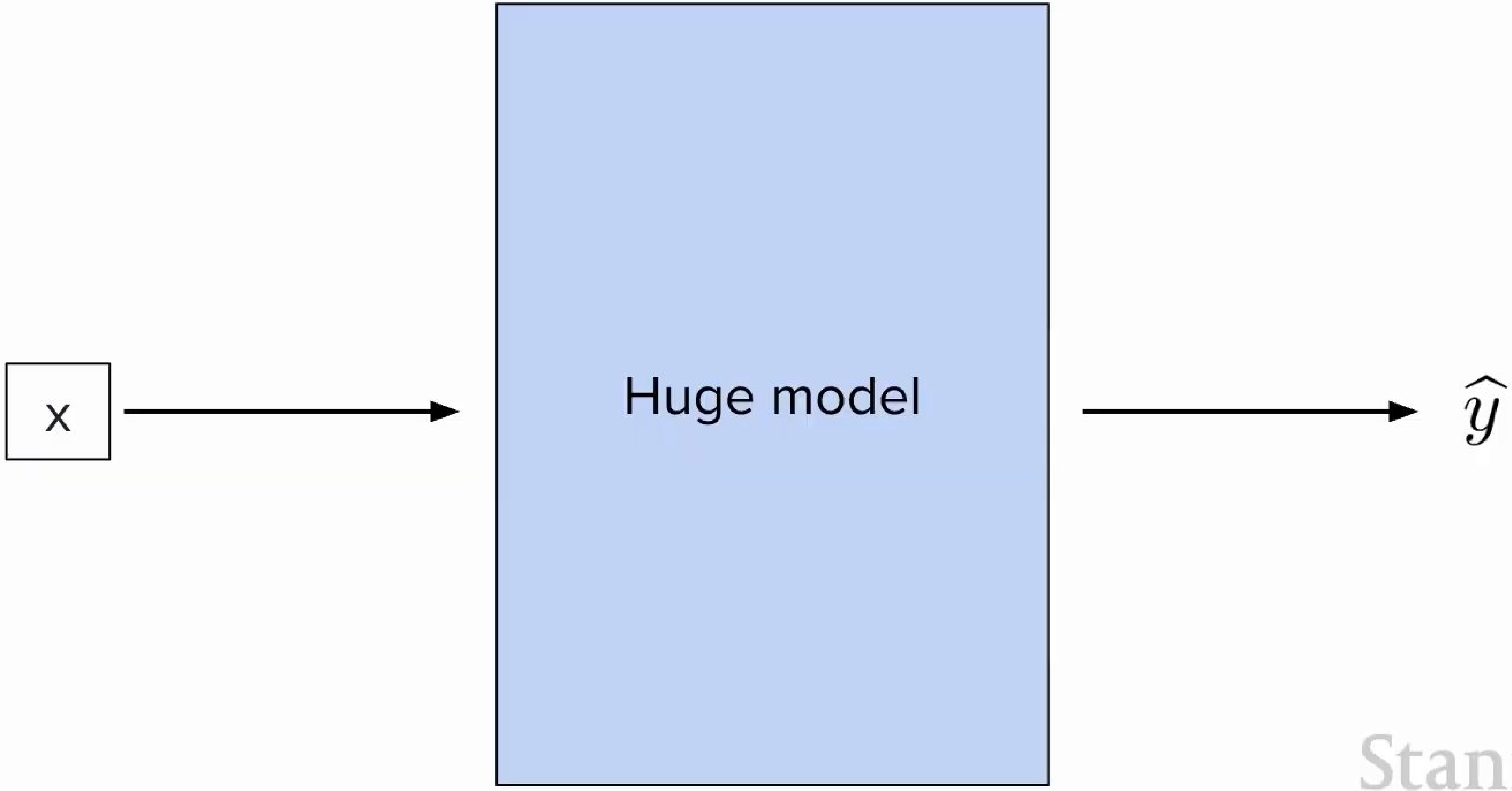
Motivation




Motivation
x
Huge model
$\hat{y}$
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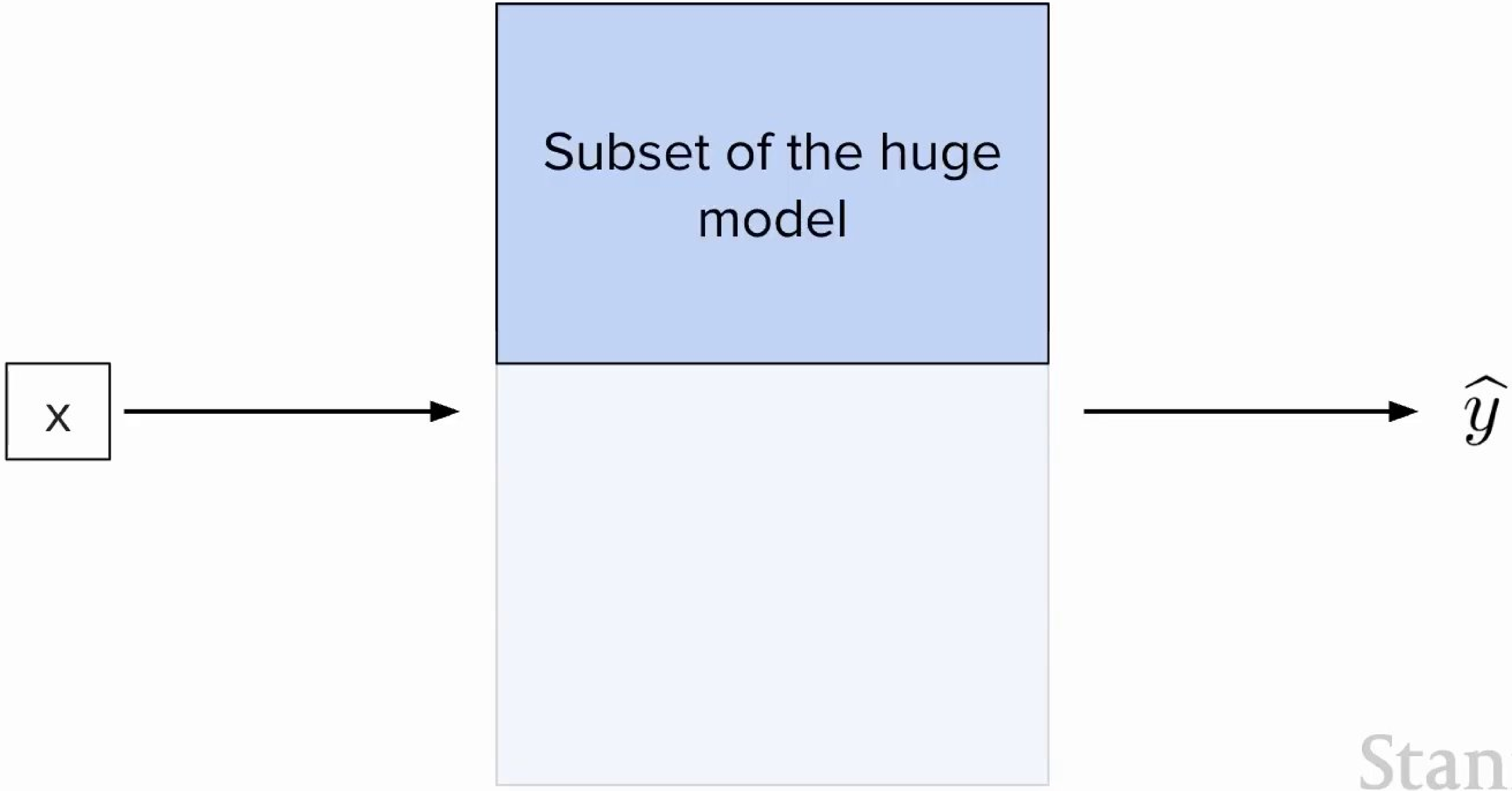
Motivation

Idea. Not all weights are useful in the forward pass




Motivation
x
E1
E2
En
ŷ
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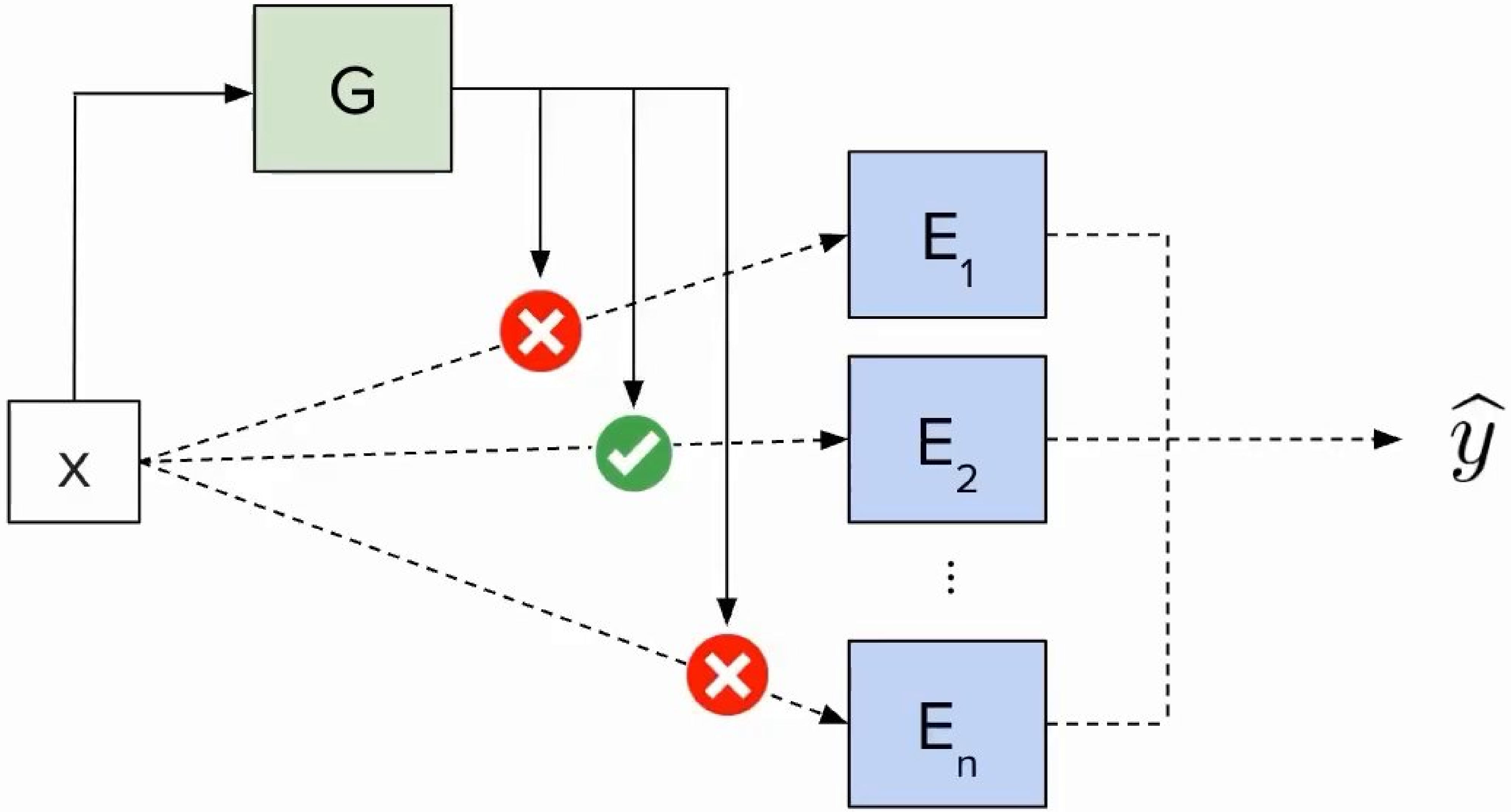
Motivation



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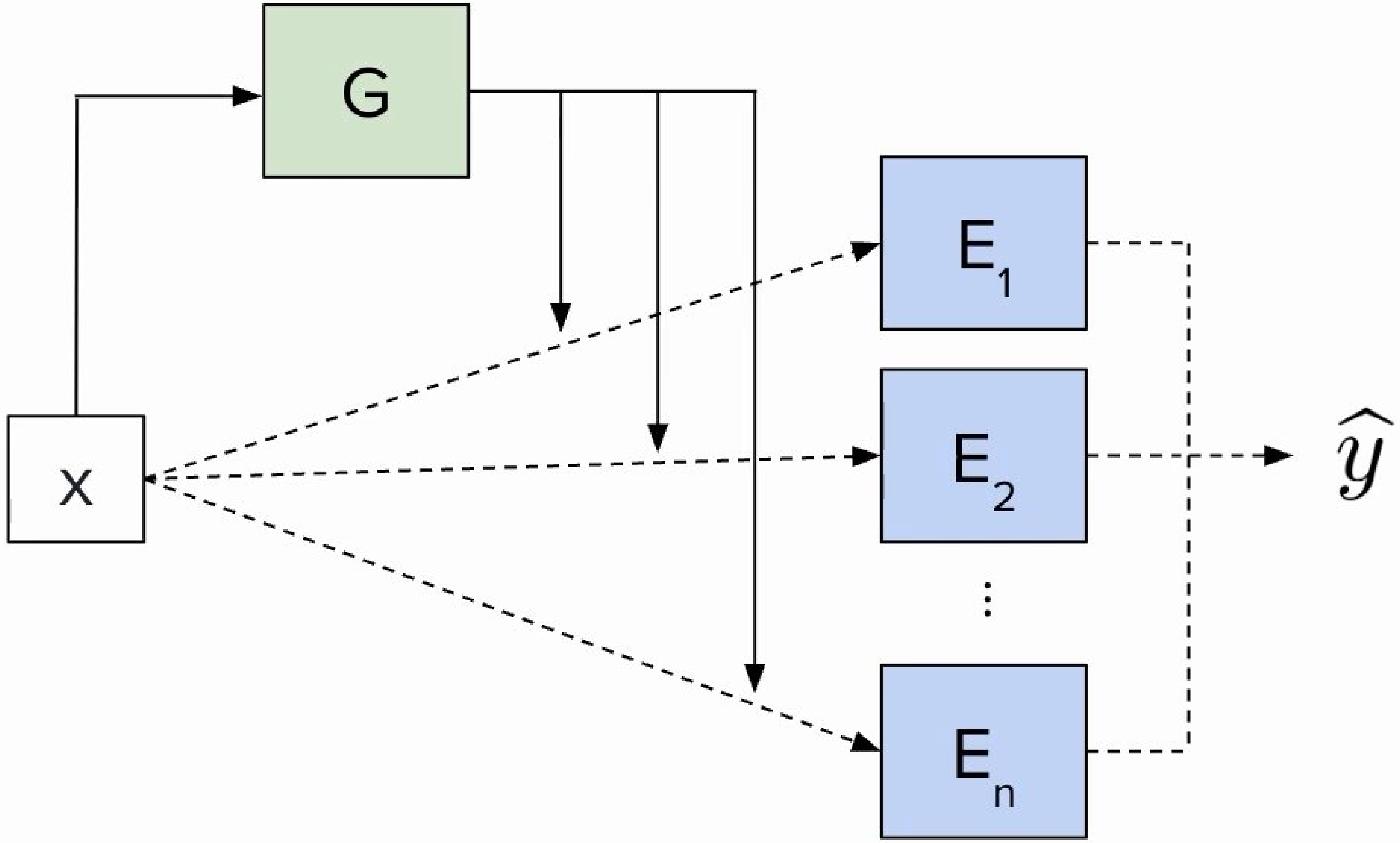
Overview of MoEs

MoE = **M**ixture **of** **E**xperts



$$\widehat{y} = \sum_{i=1}^{n} G(x)_i E_i(x)$$

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Overview of MoEs
MoE = Mixture of Experts
G
x
E_1
E_2
E_n
$\widehat{y}$
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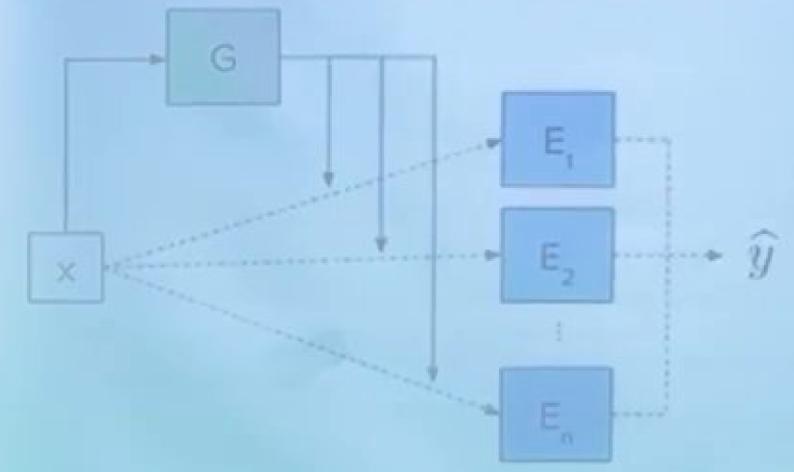

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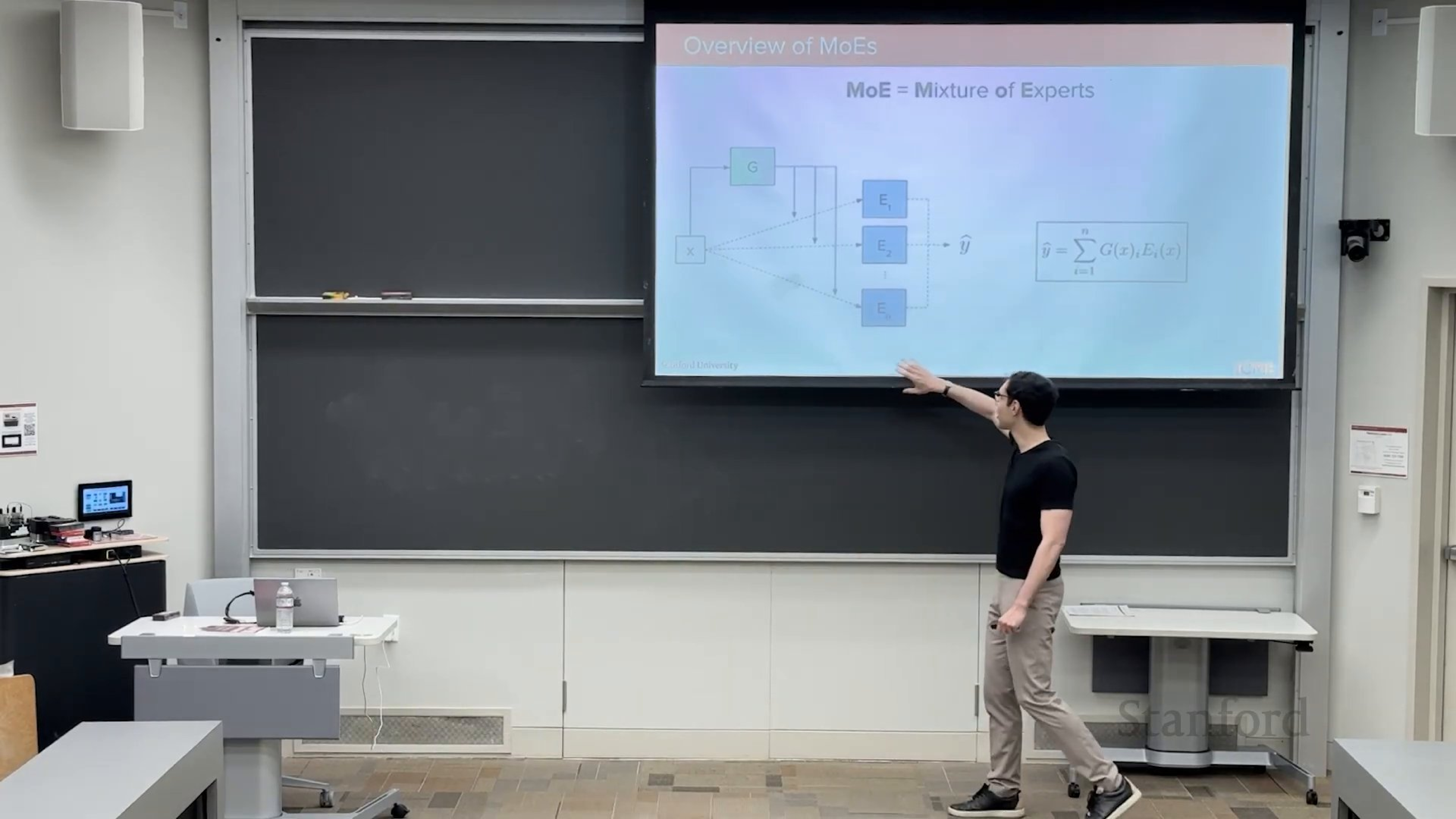
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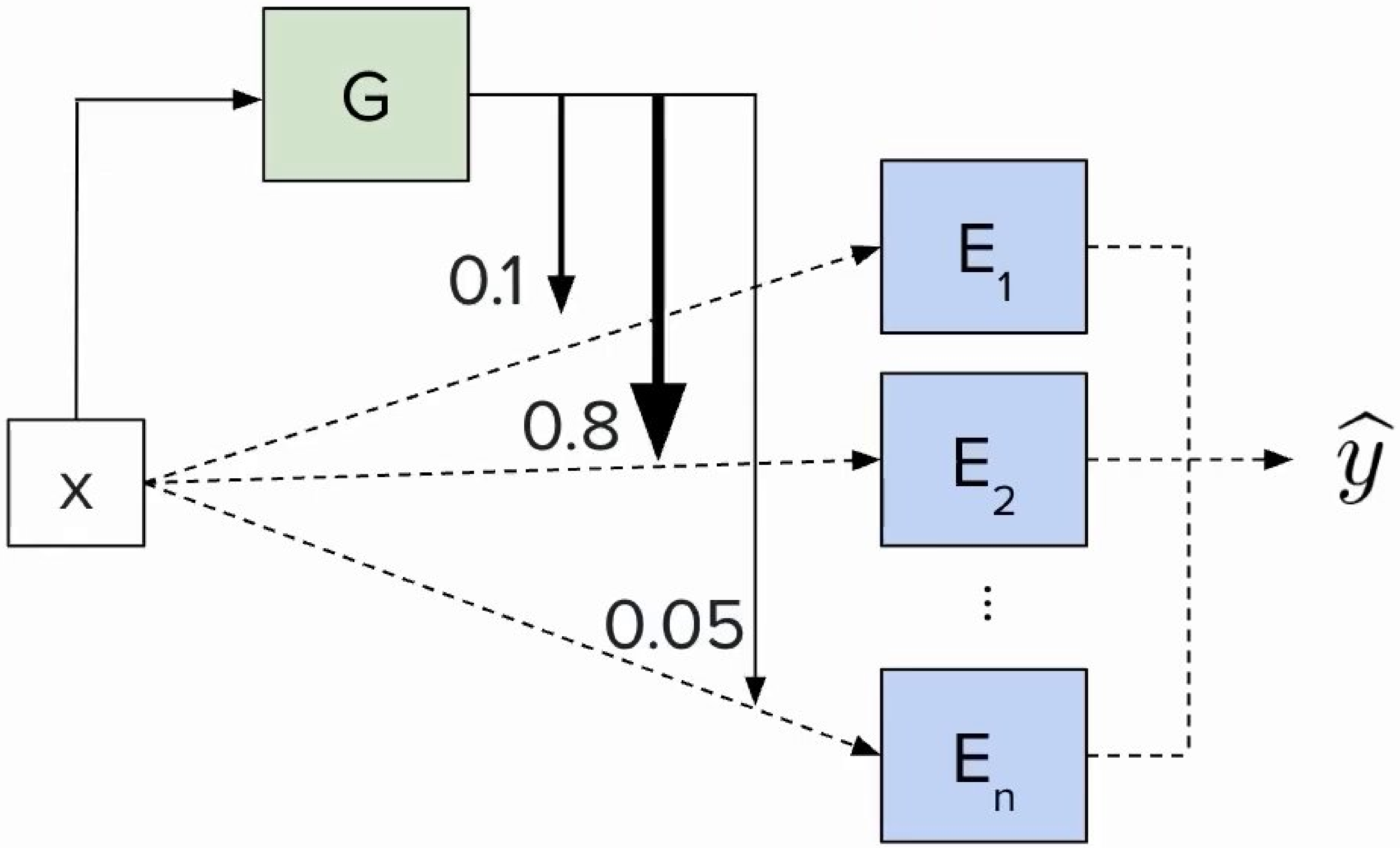

Dense MoE. Output is weighted average of **all** expert outputs.

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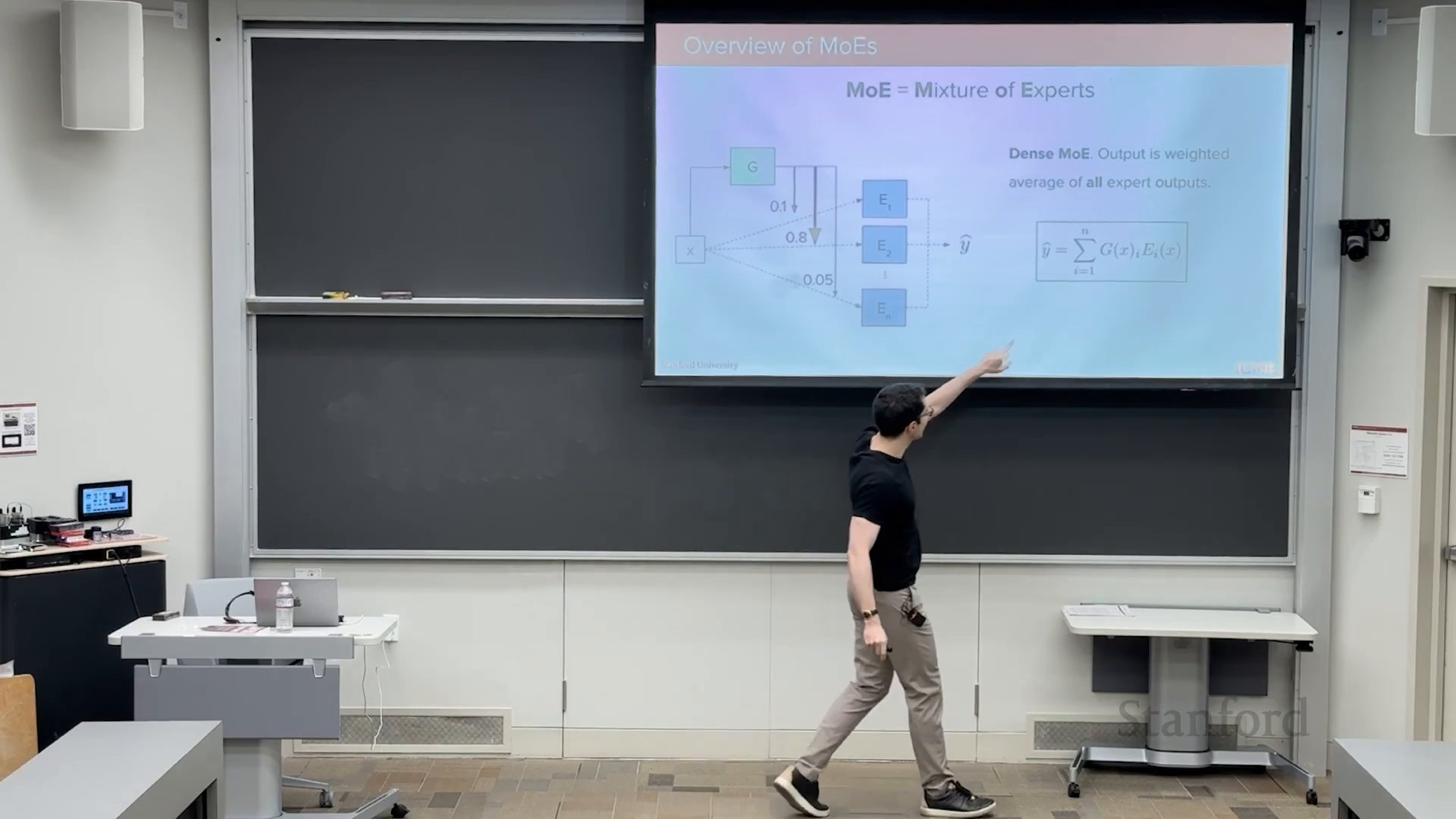

Overview of MoEs
MoE = Mixture of Experts
G
0.1
0.8
0.05
x
E1
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ŷ
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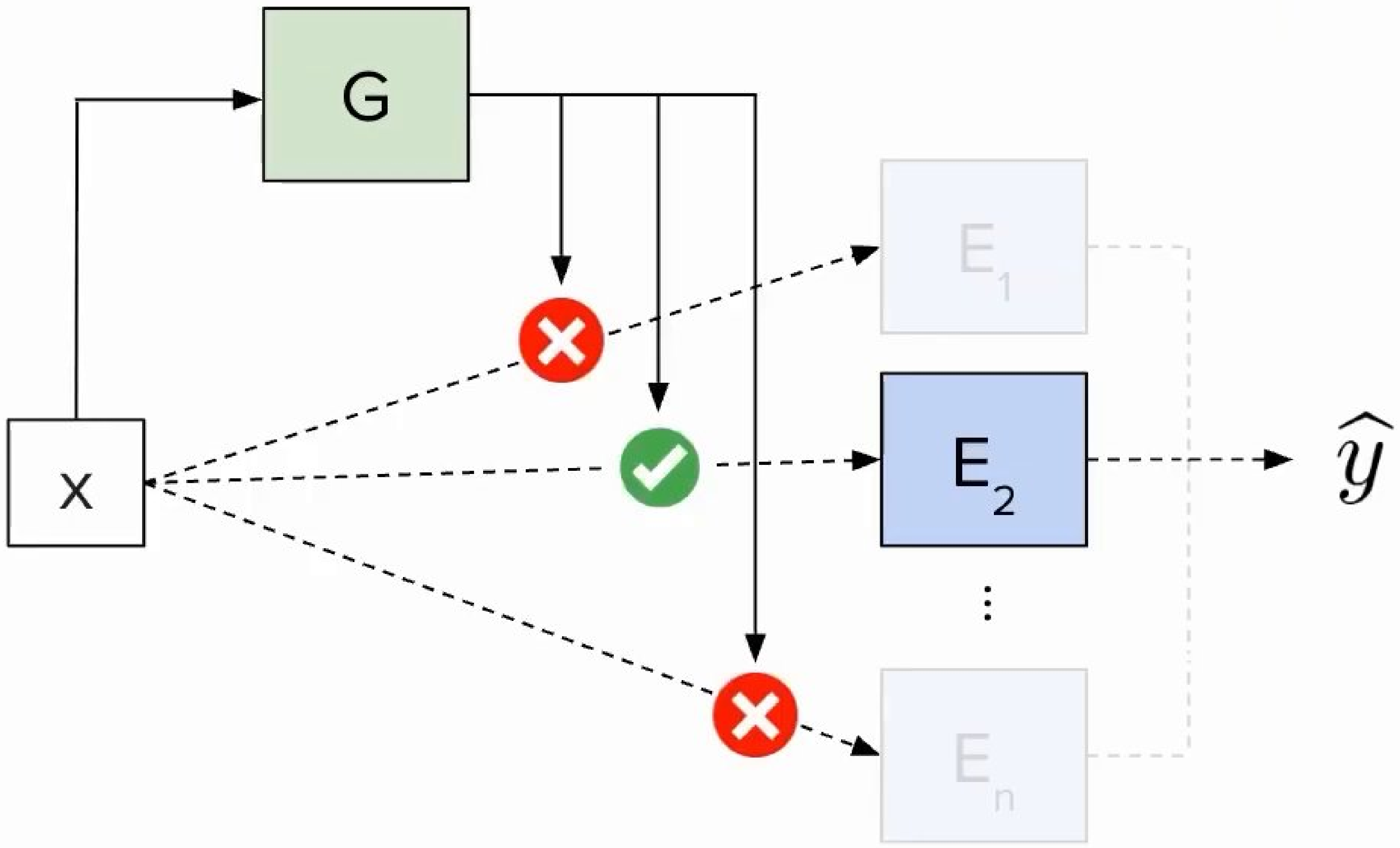

Sparse MoE. Output is weighted average of **selected** expert outputs.

$$\hat{y} = \sum_{i \in \mathcal{I}_k} G(x)_i E_i(x)$$

Via **top-k** selection


Overview of MoEs
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x
E2
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Via top-k selection
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"The Sparsely-Gated Mixture-of-Experts Layer", Shazeer et al., 2017
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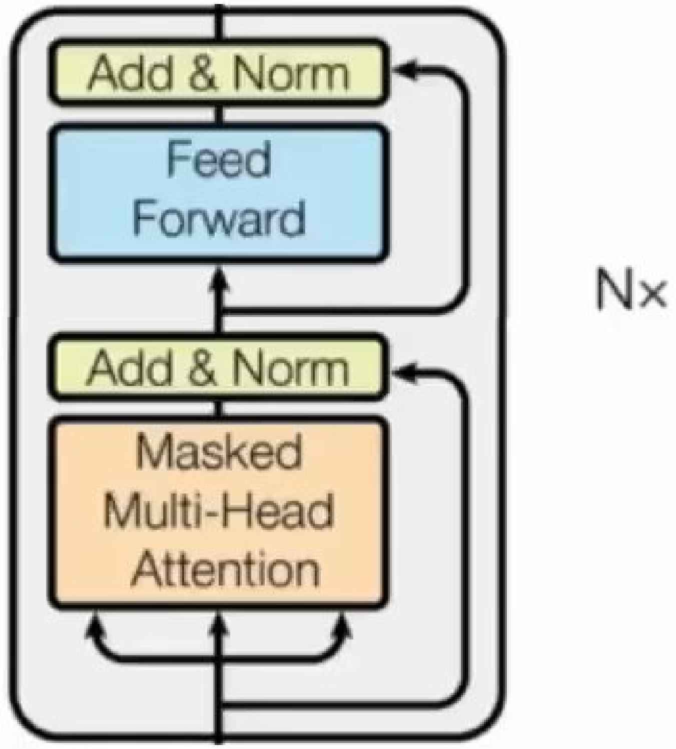
MoE in Transformer-based models



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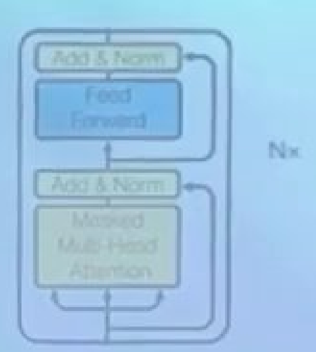

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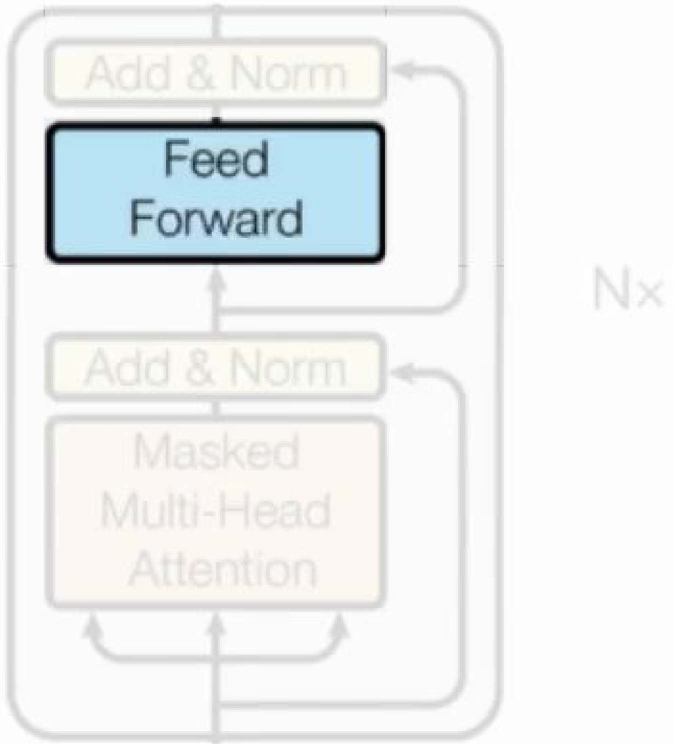

Routing done **for each token**!

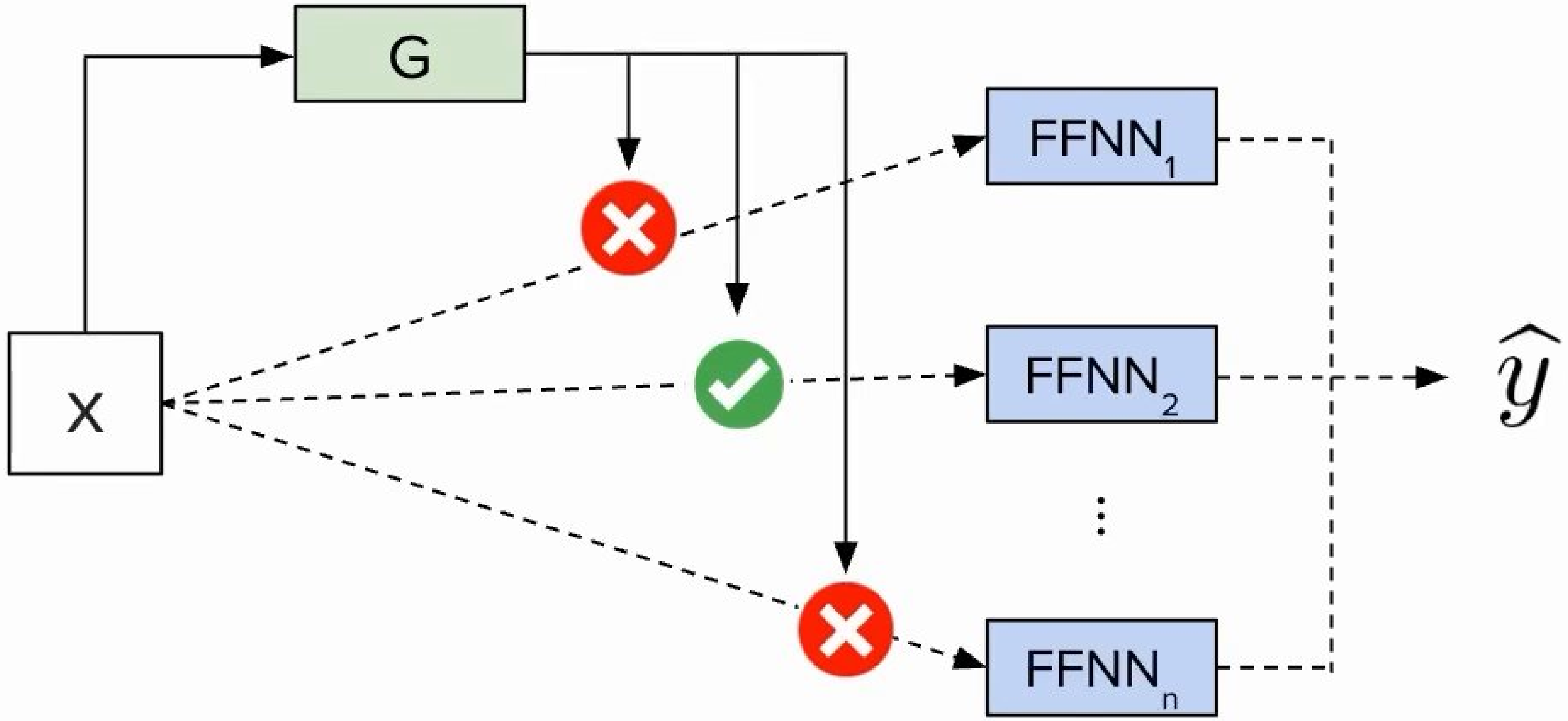

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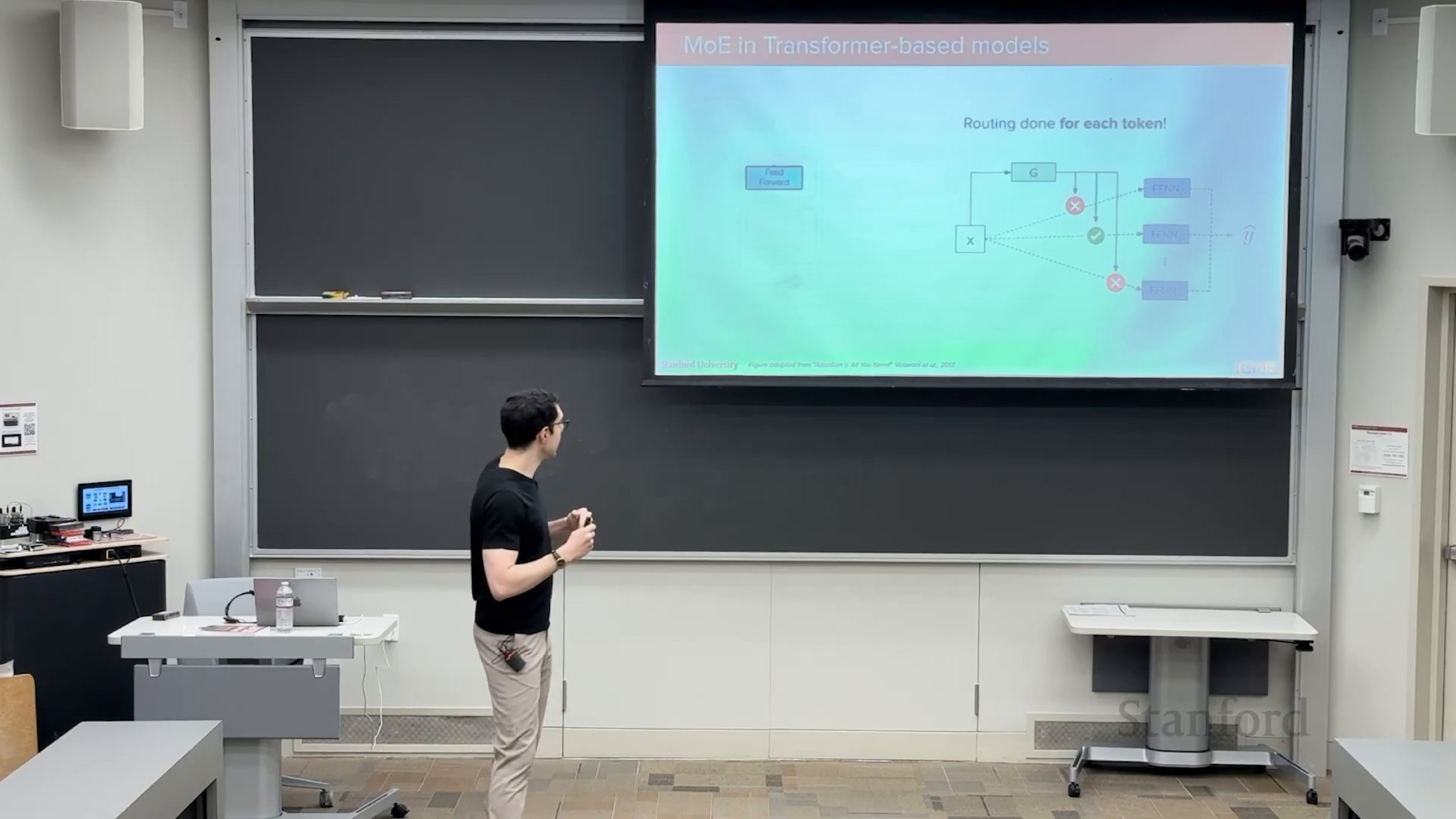
Figure adapted from "Attention is All You Need", Vaswani et al., 2017.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Feed Forward
G
x
FFNN
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Training challenges include routing collap

Symptom. Same expert gets selected most of the time.

"routing collapse"

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 "Switch Transformers: Scaling to Trillion Parameter Models with Simple and Efficient Sparsity", Fedus et al., 2021.


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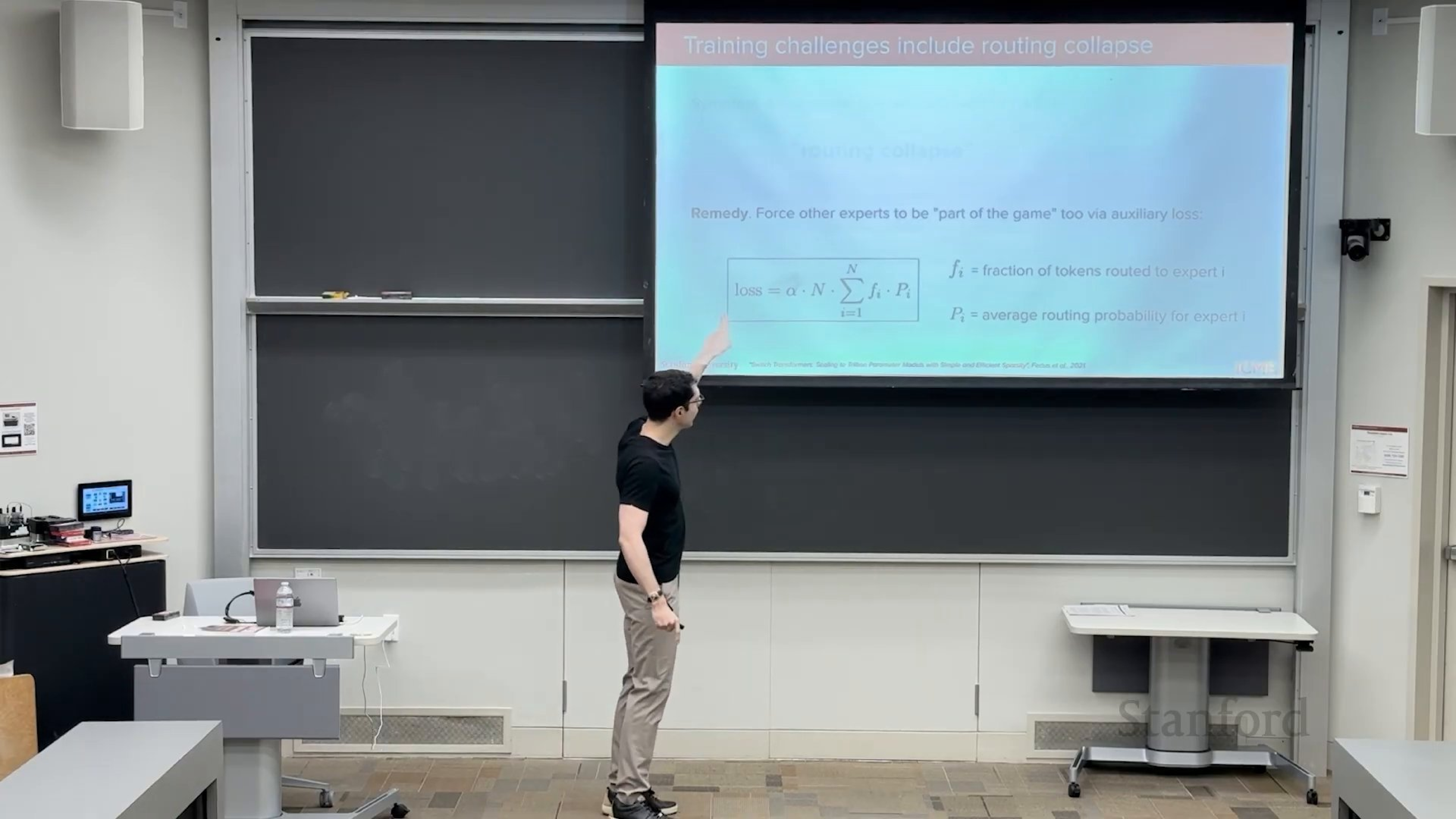

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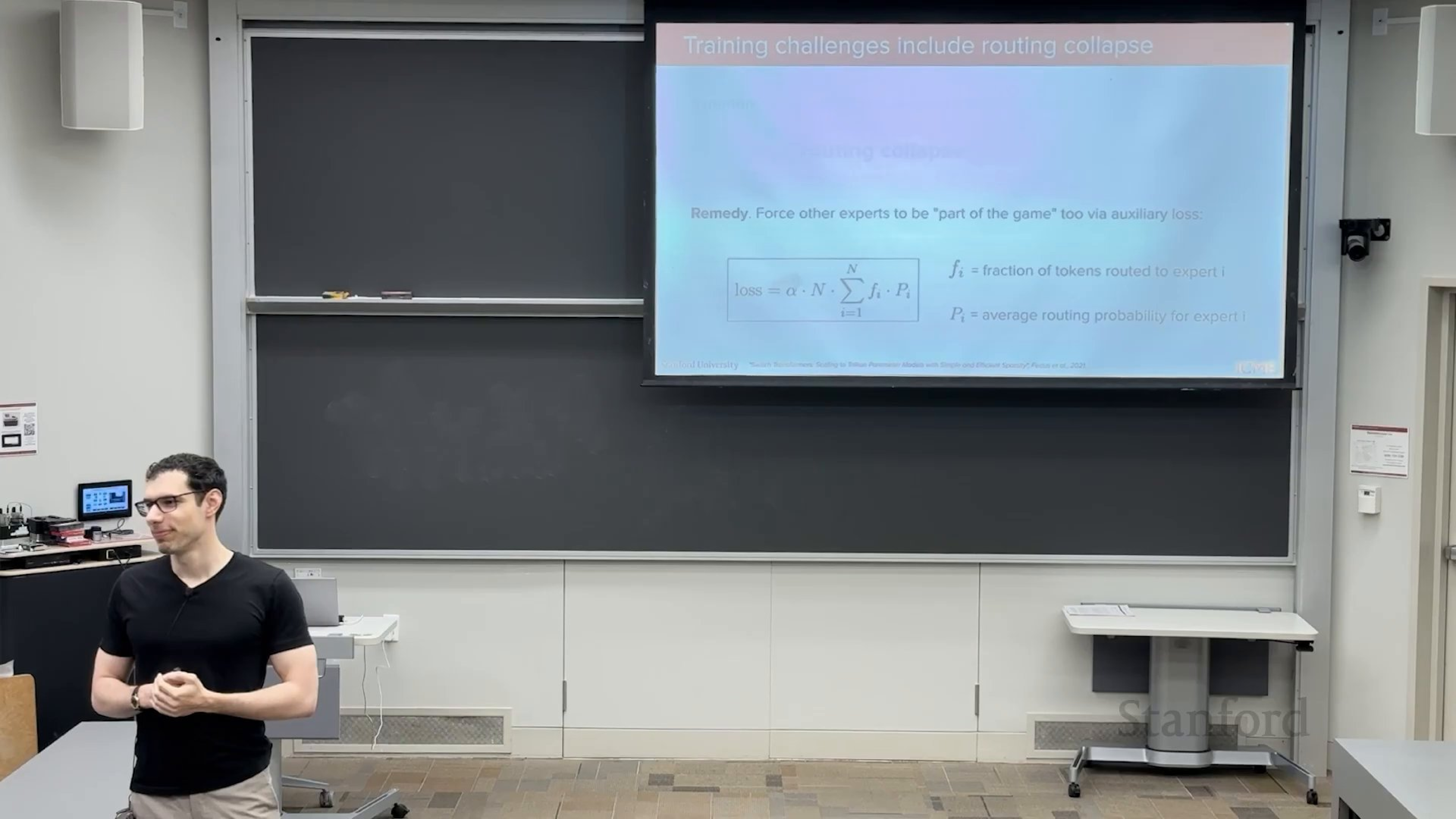
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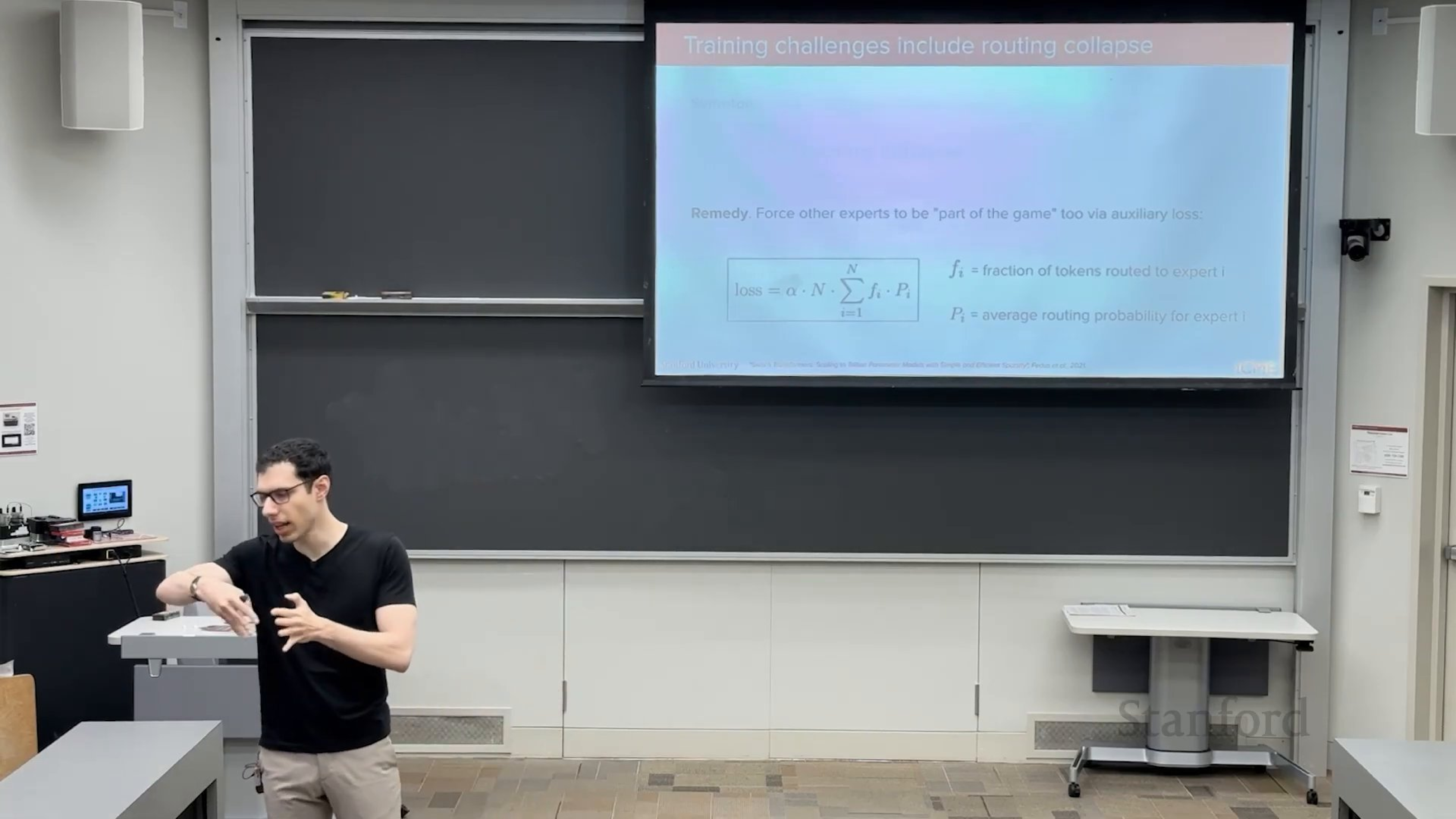
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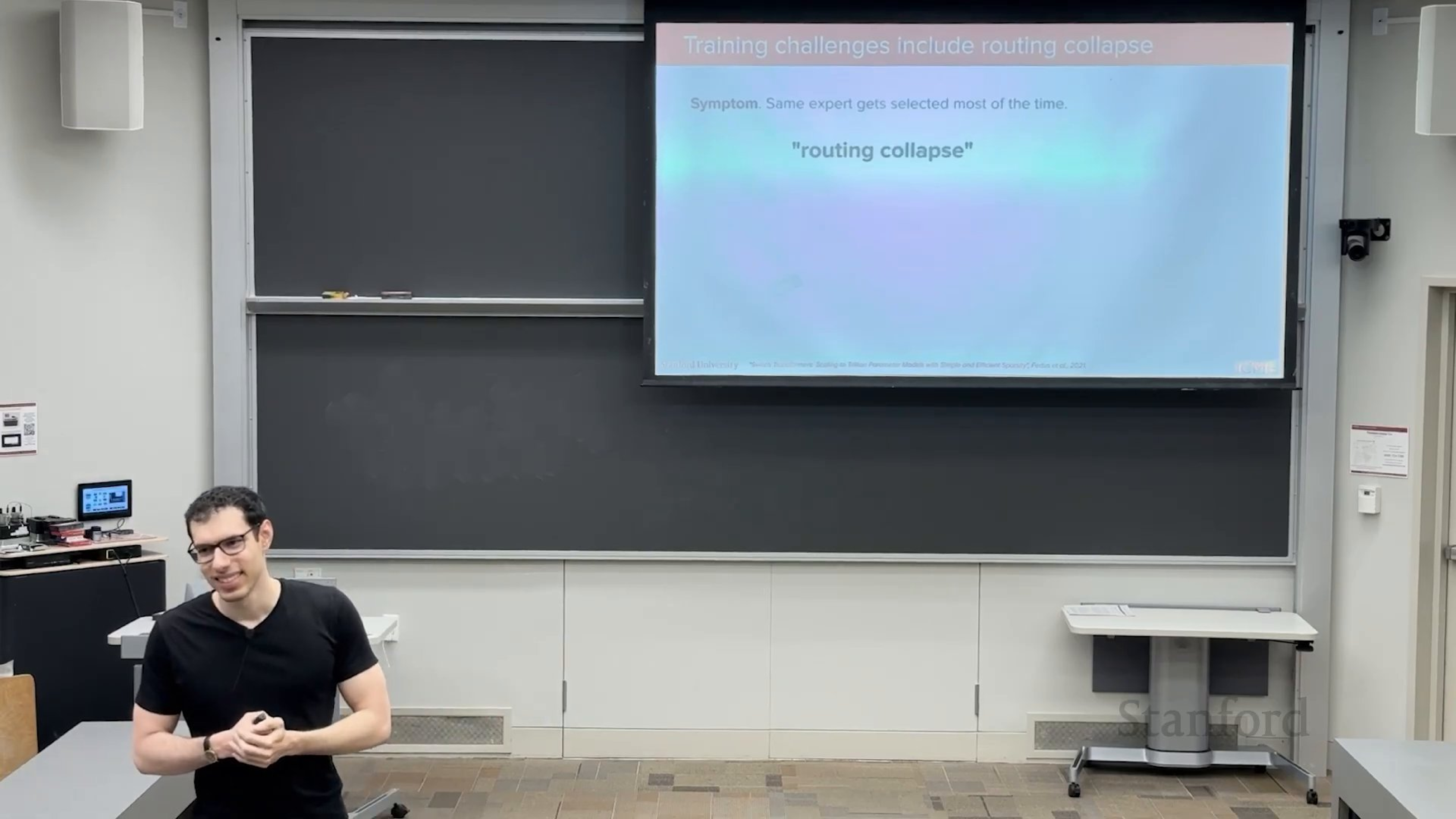
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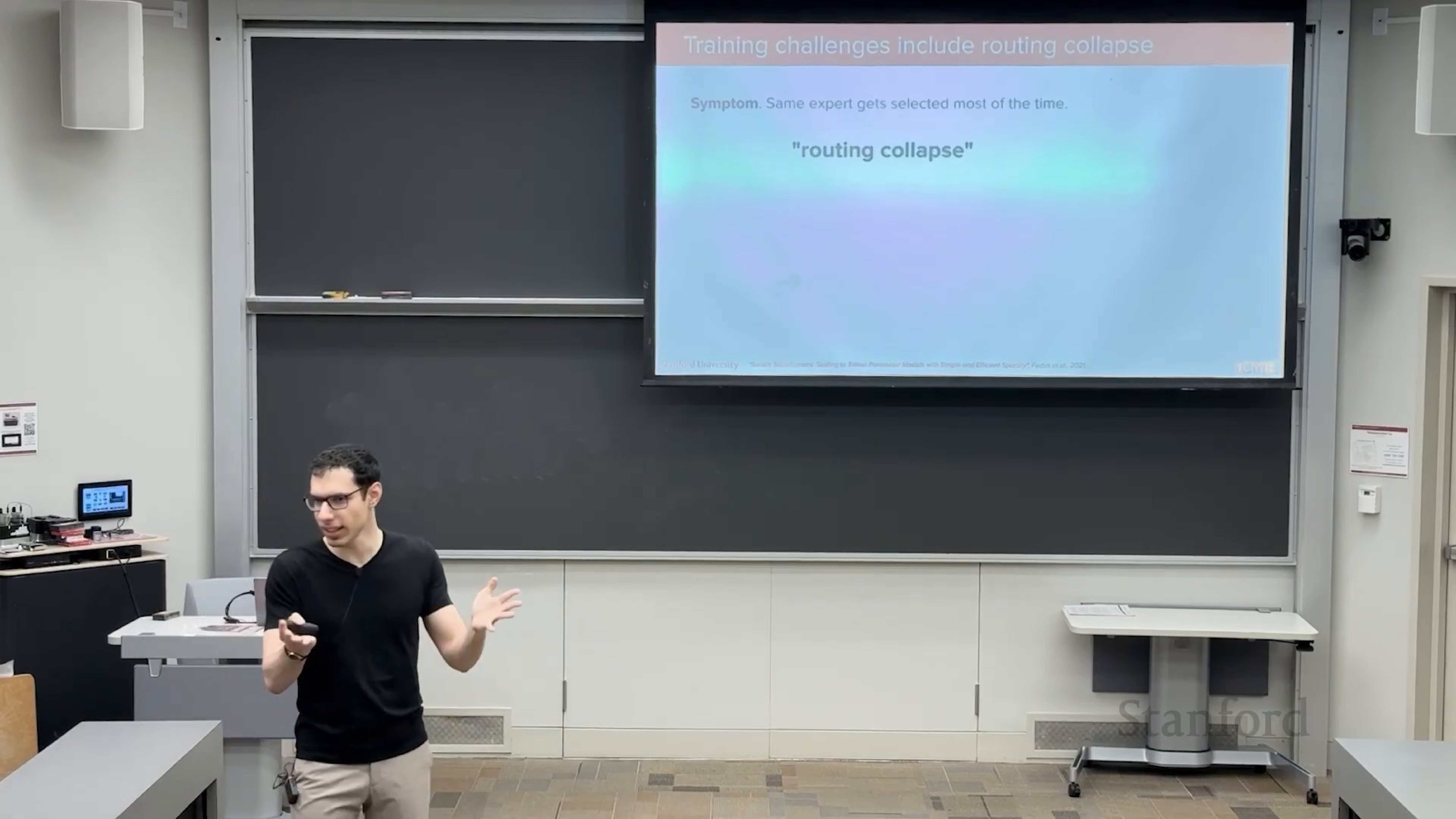
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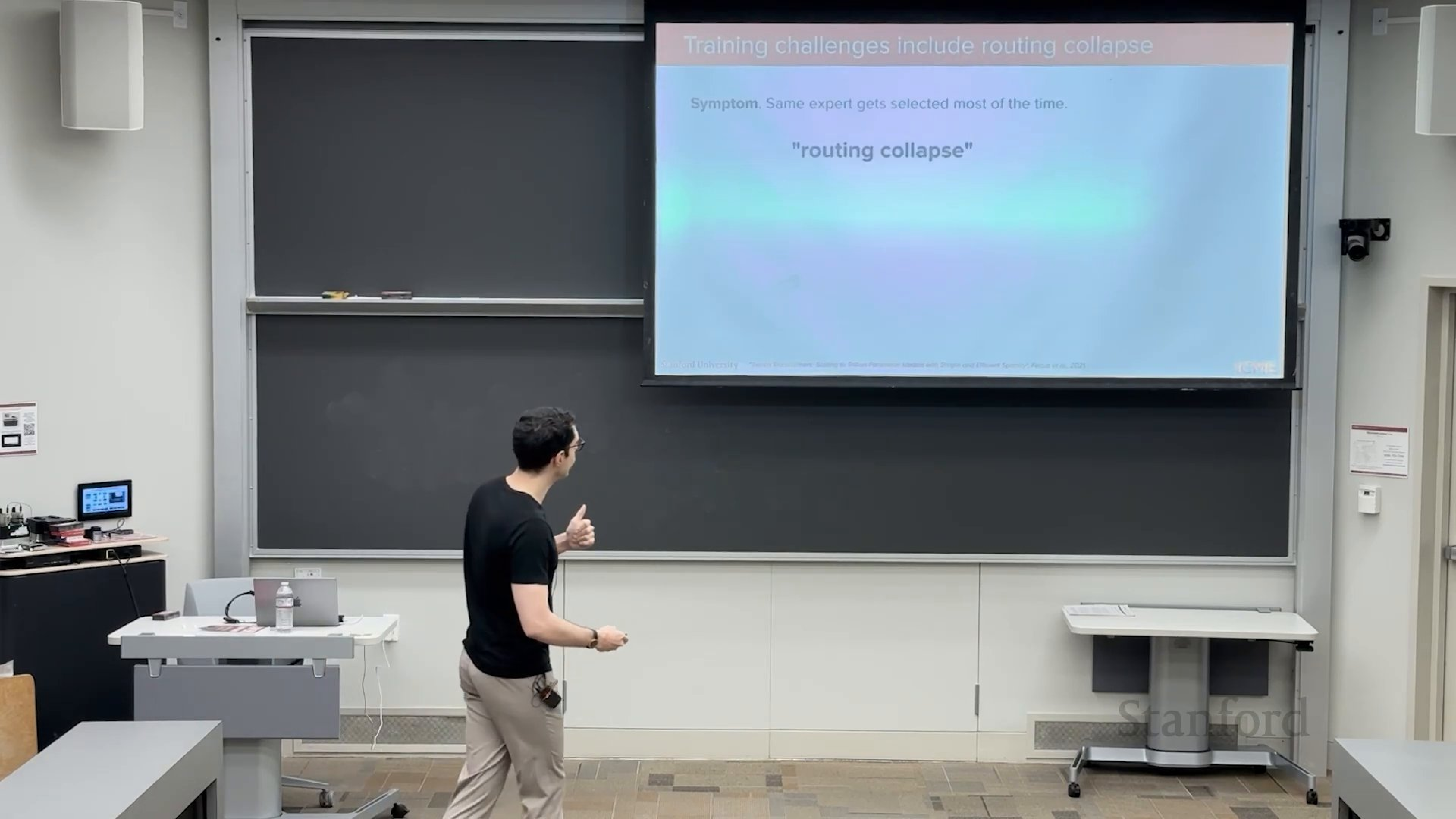
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MoE in Transformer-based models
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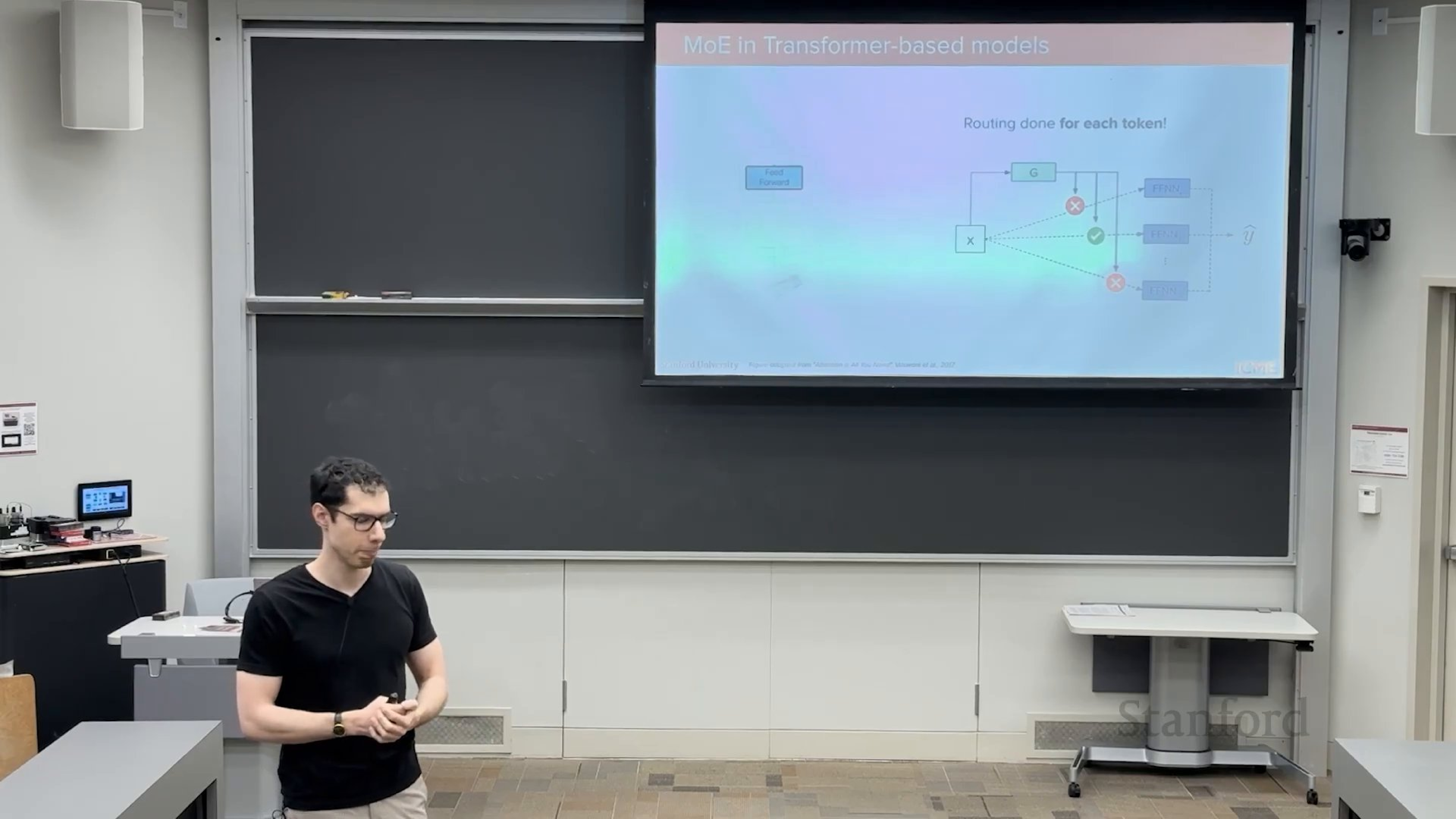
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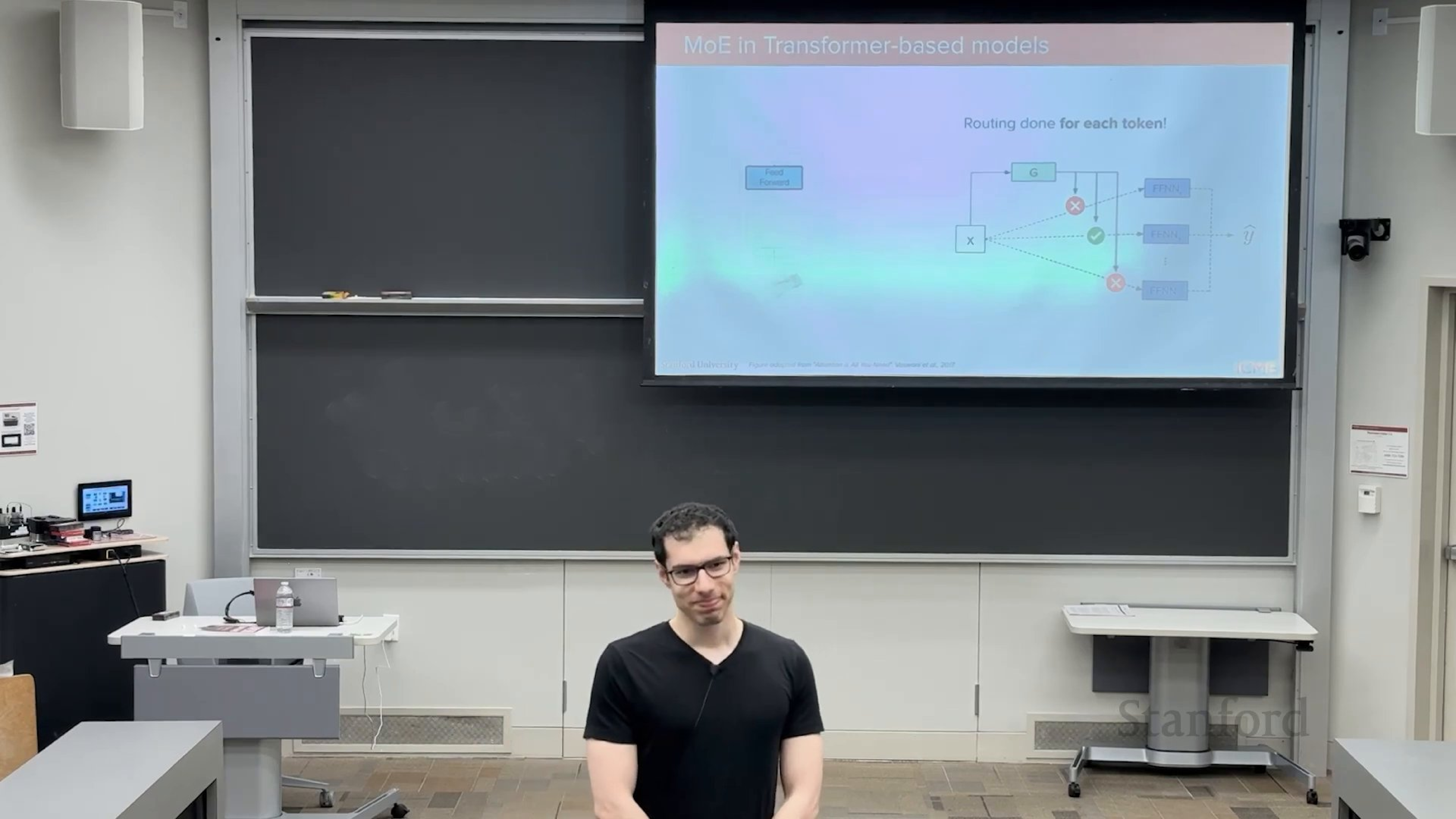
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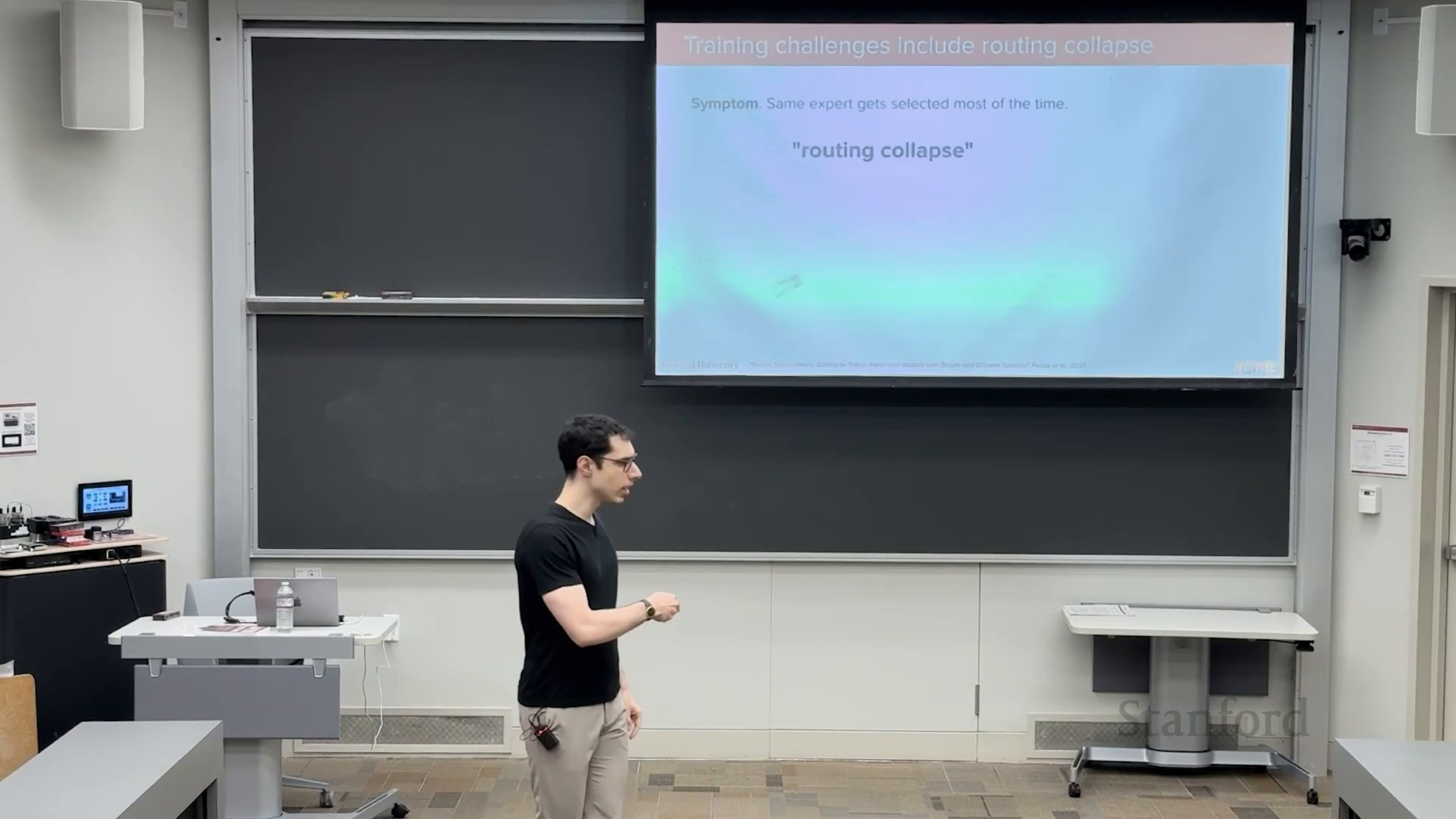
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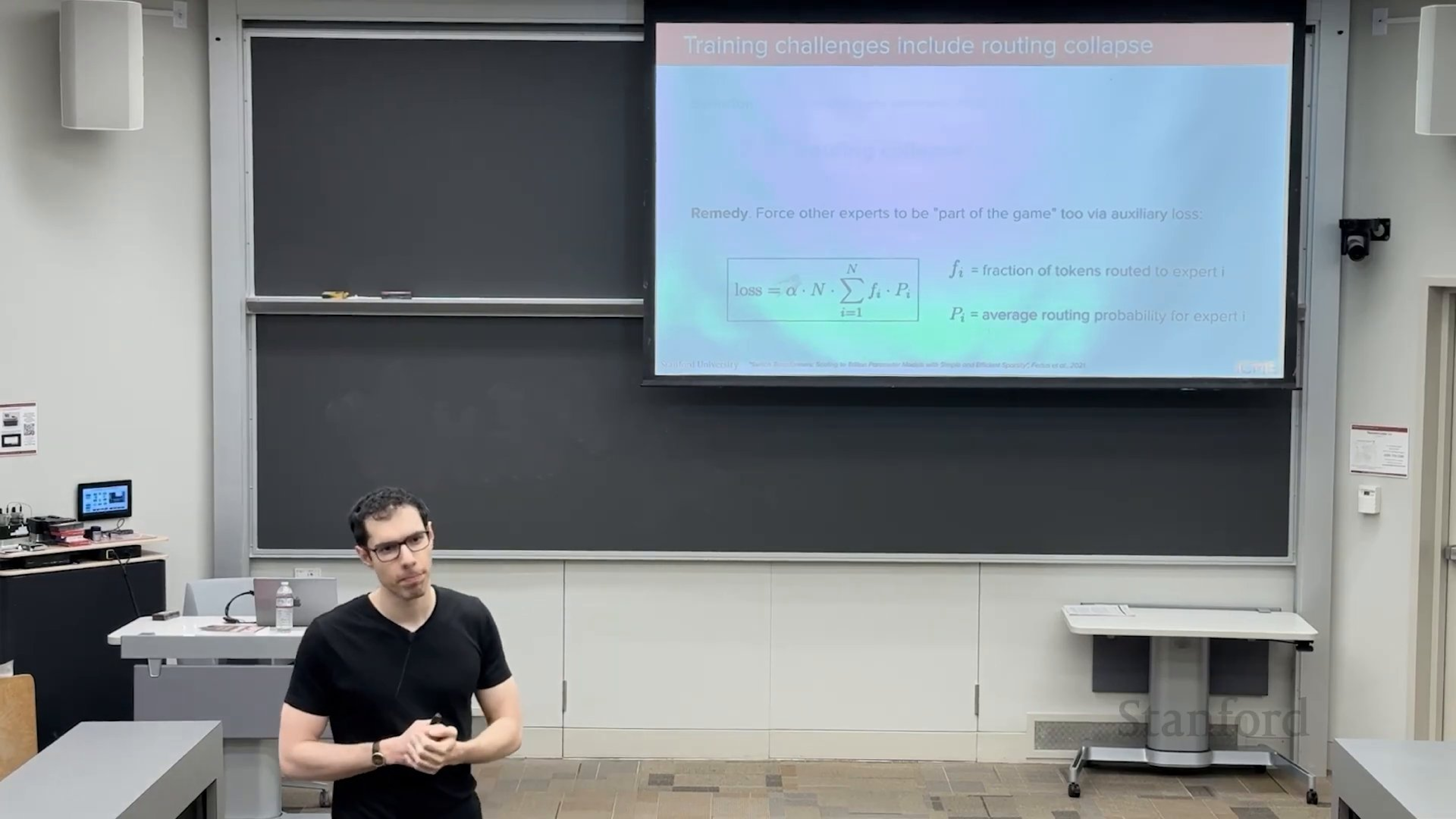
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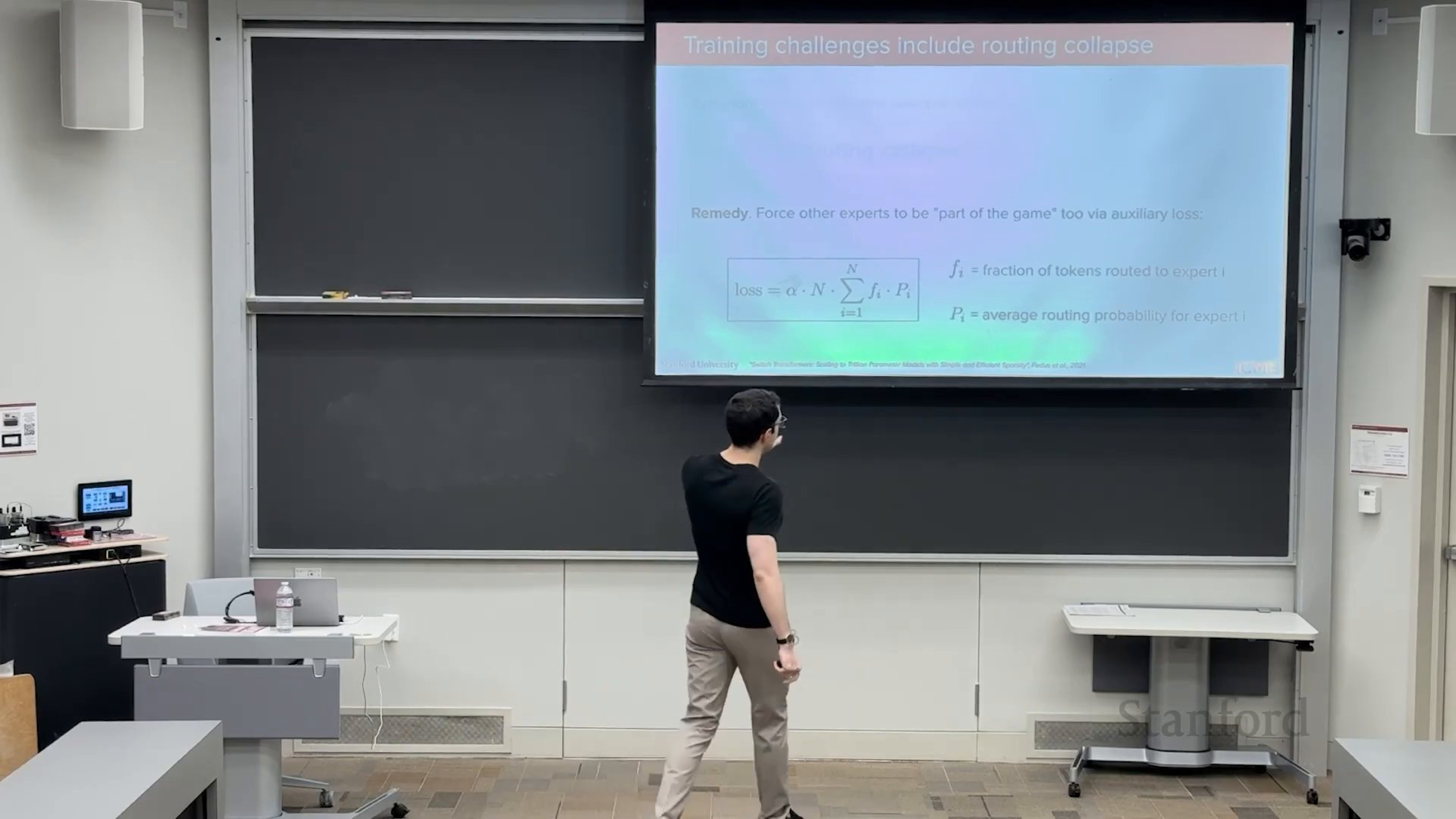
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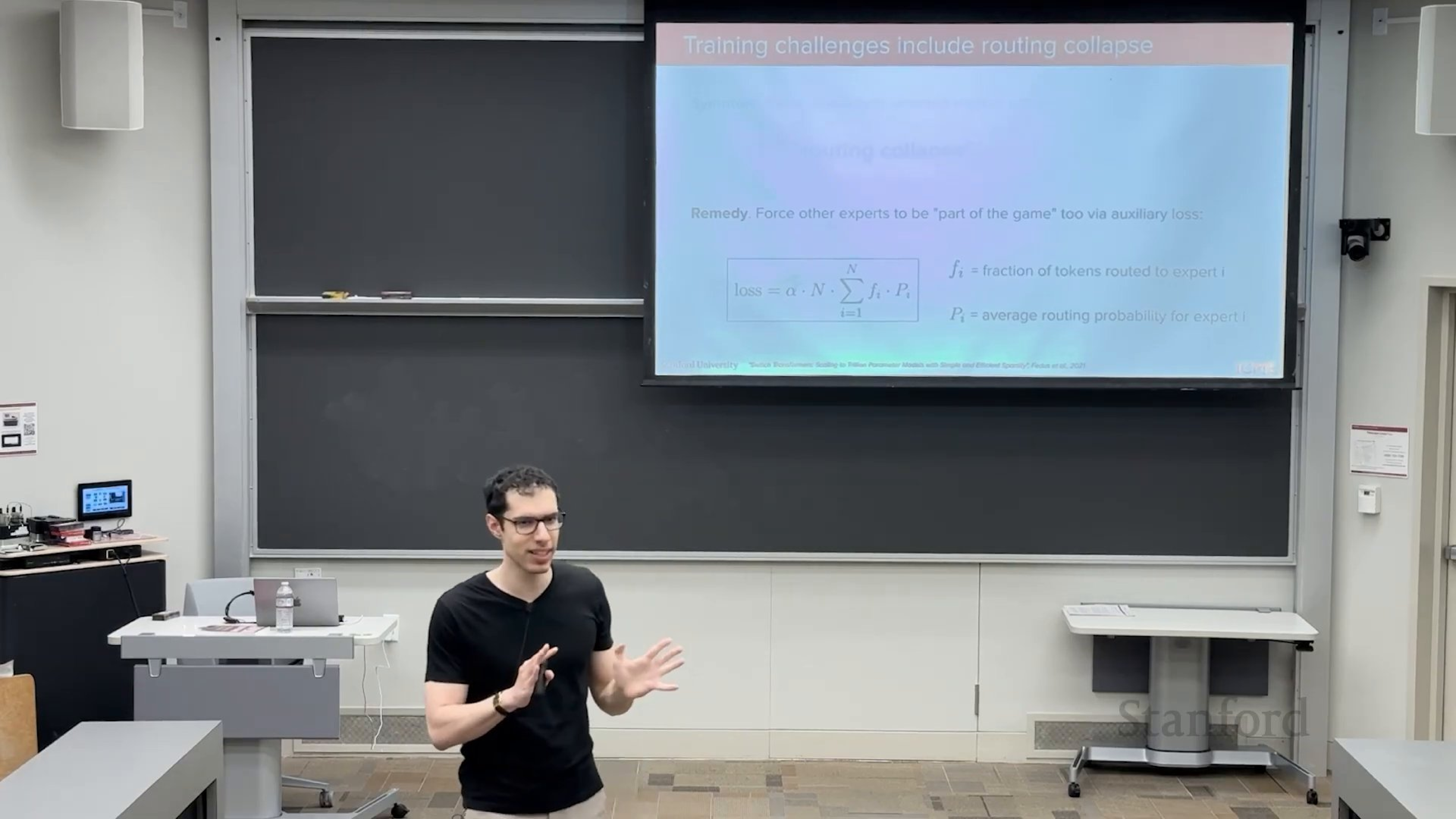
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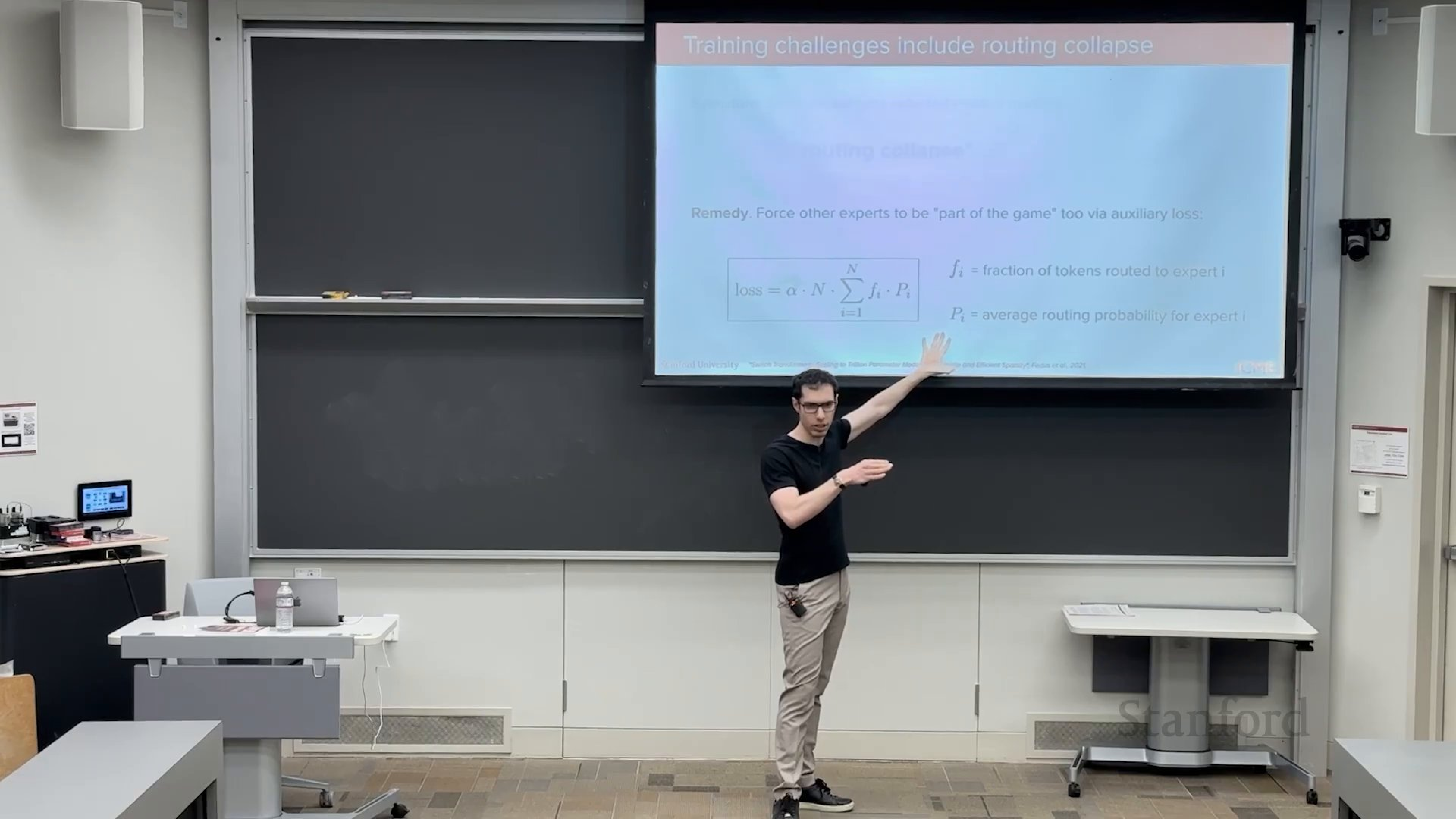
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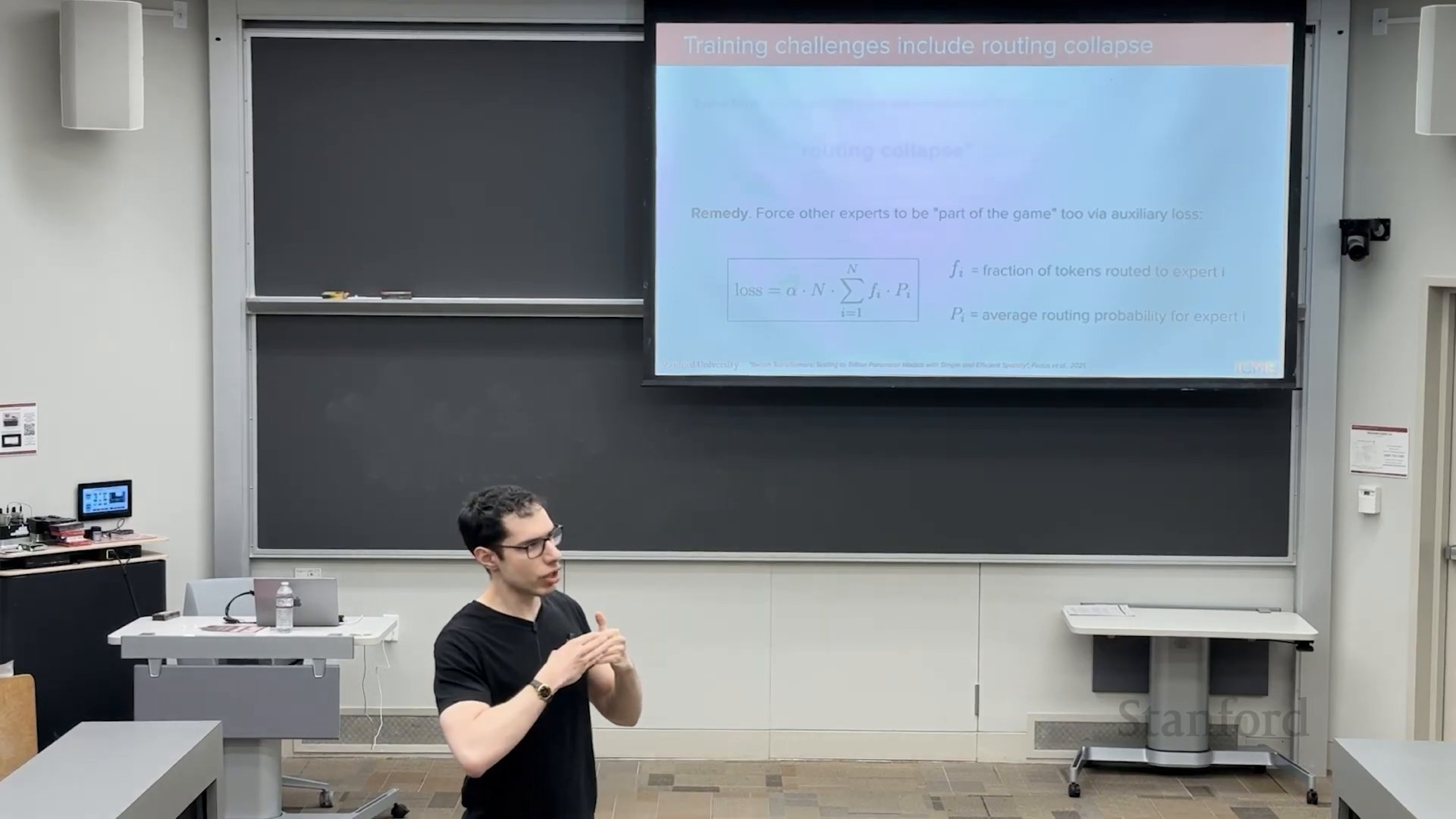
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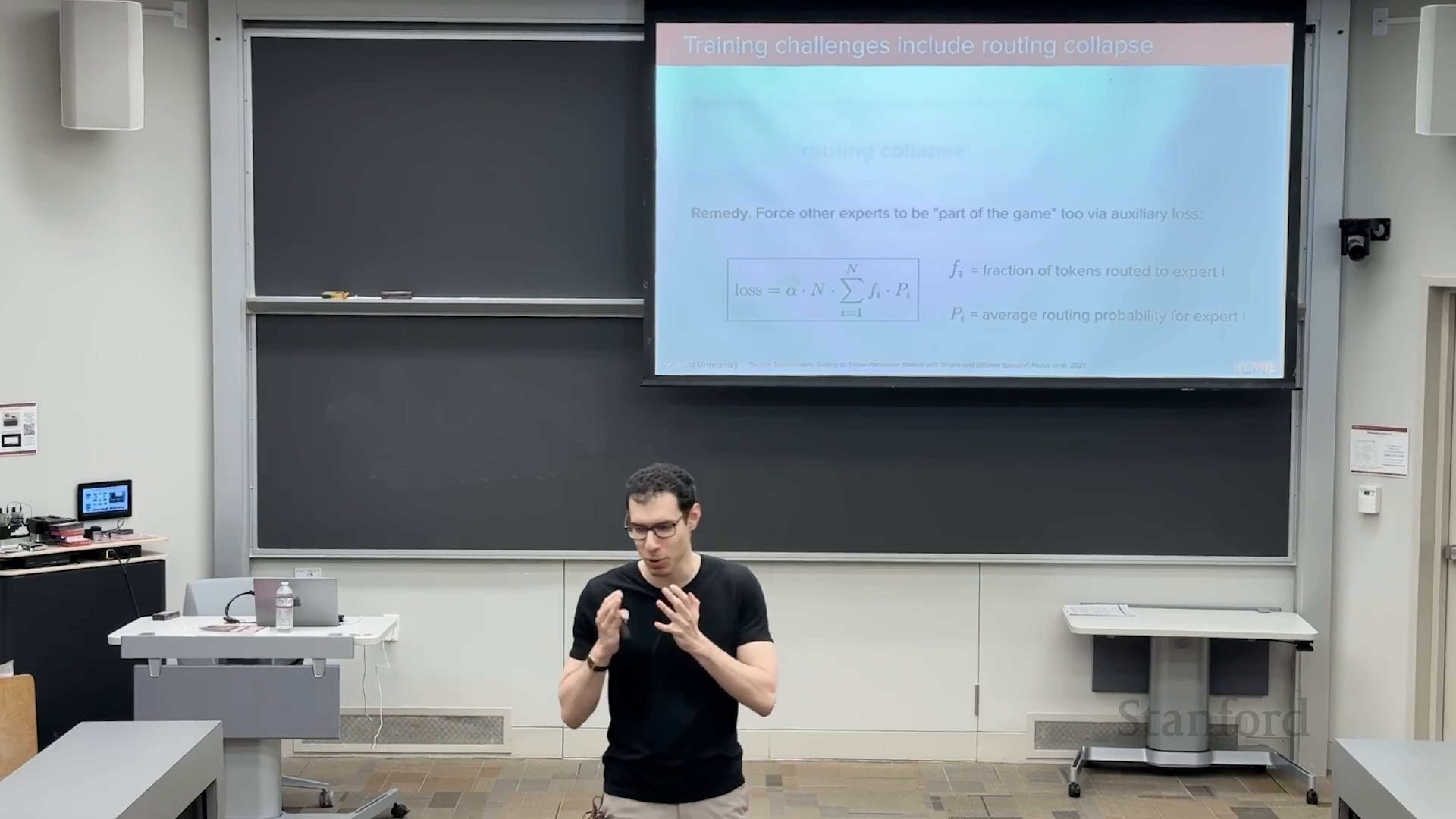
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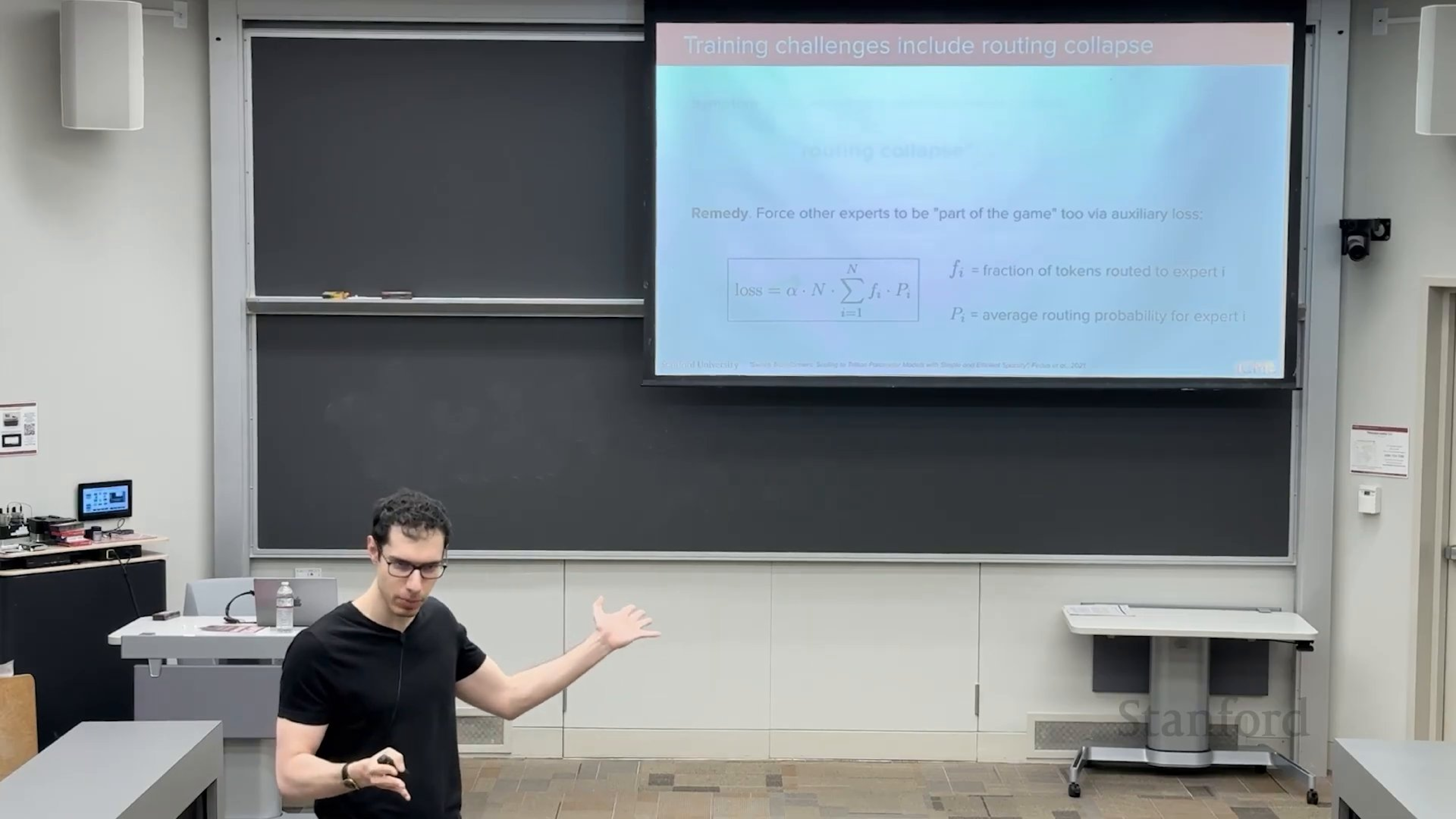
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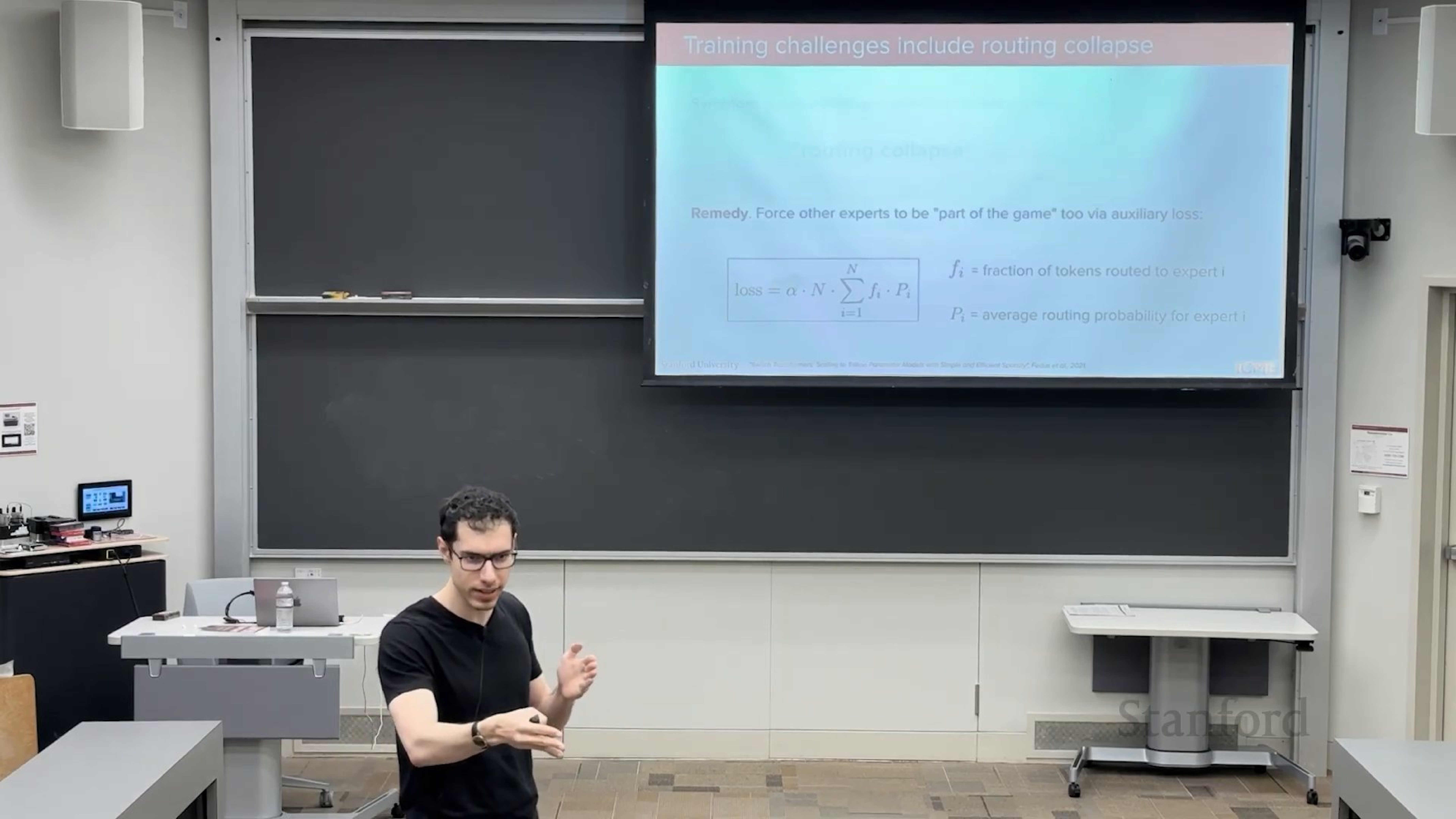
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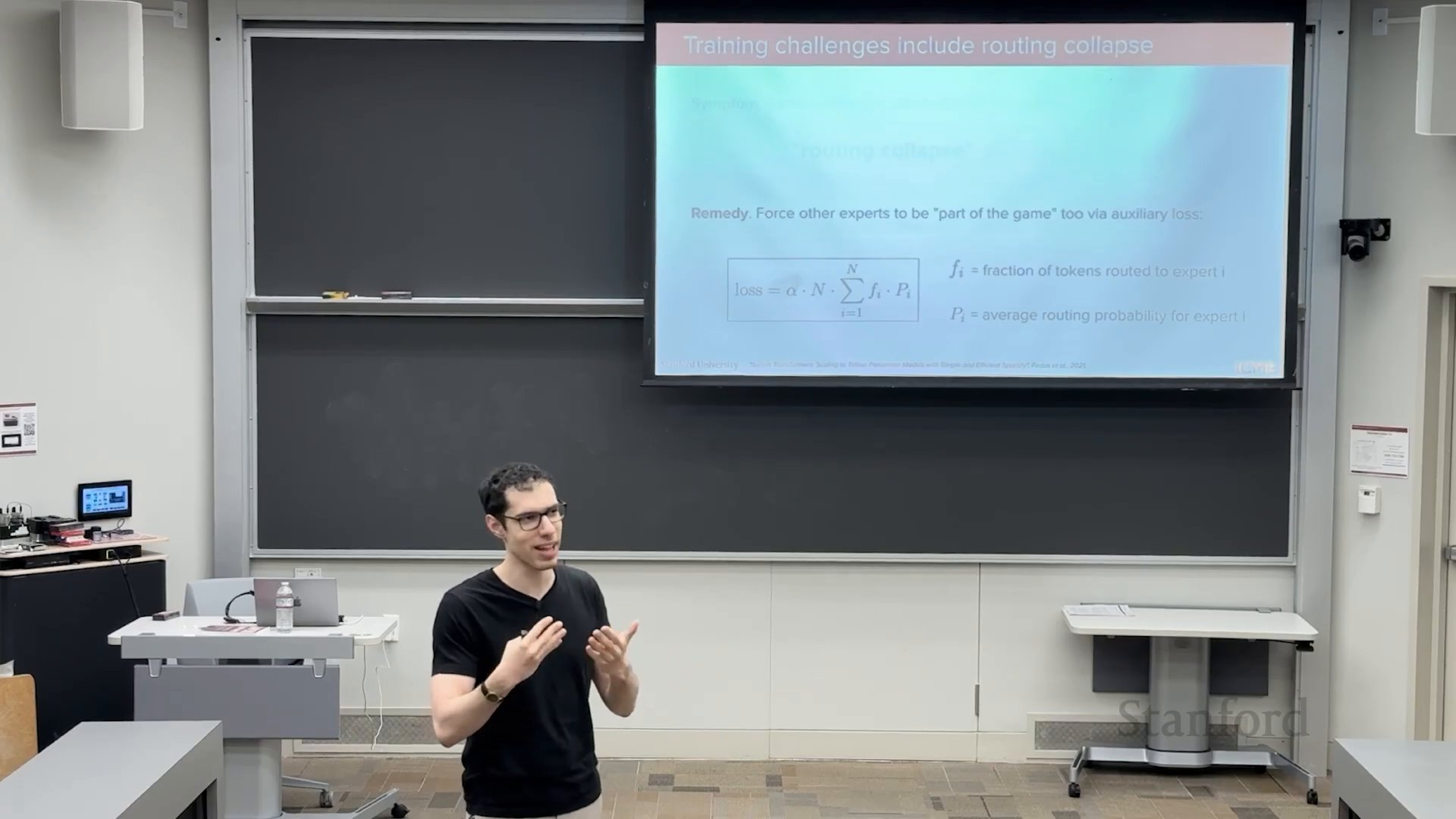

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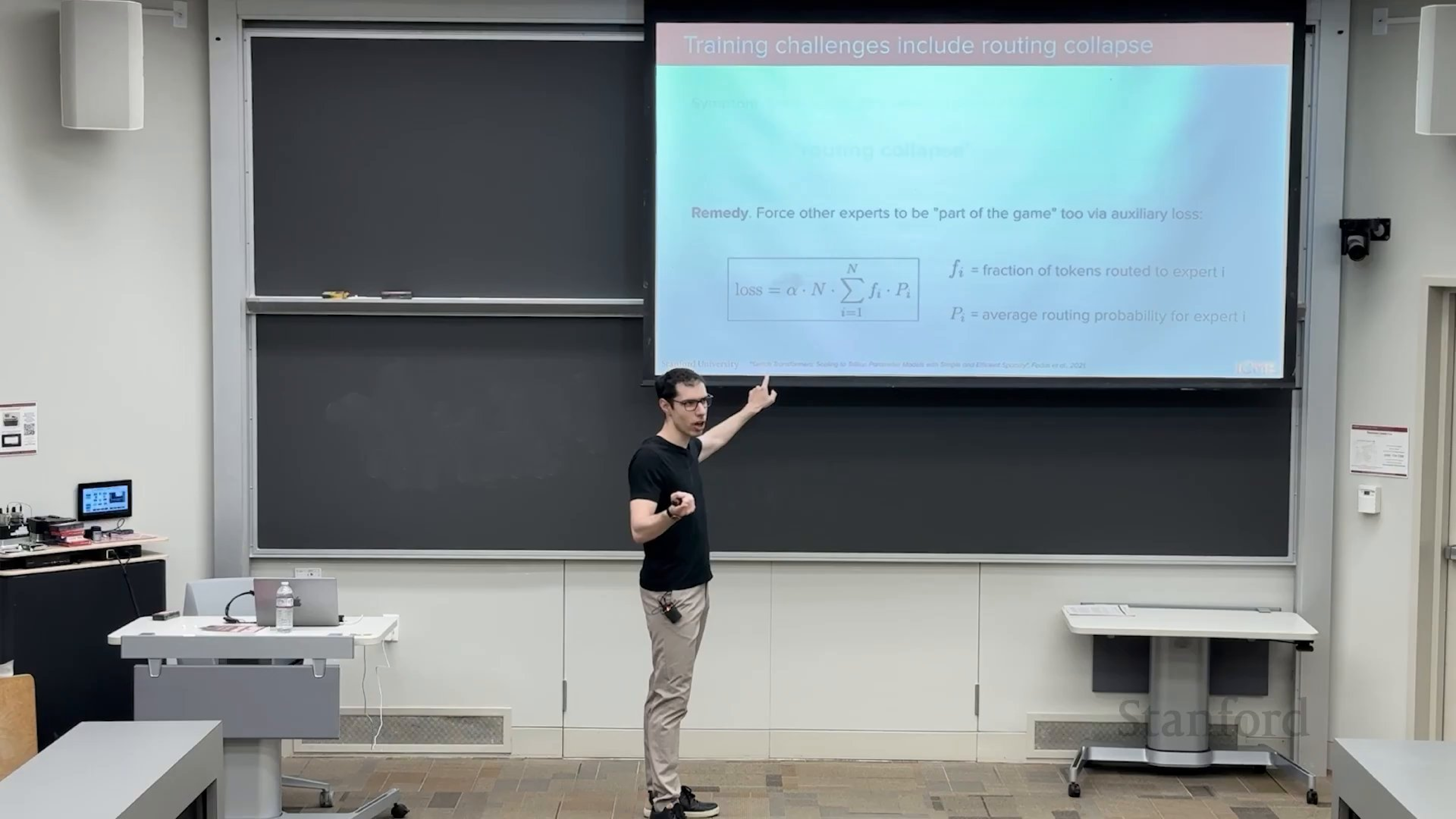

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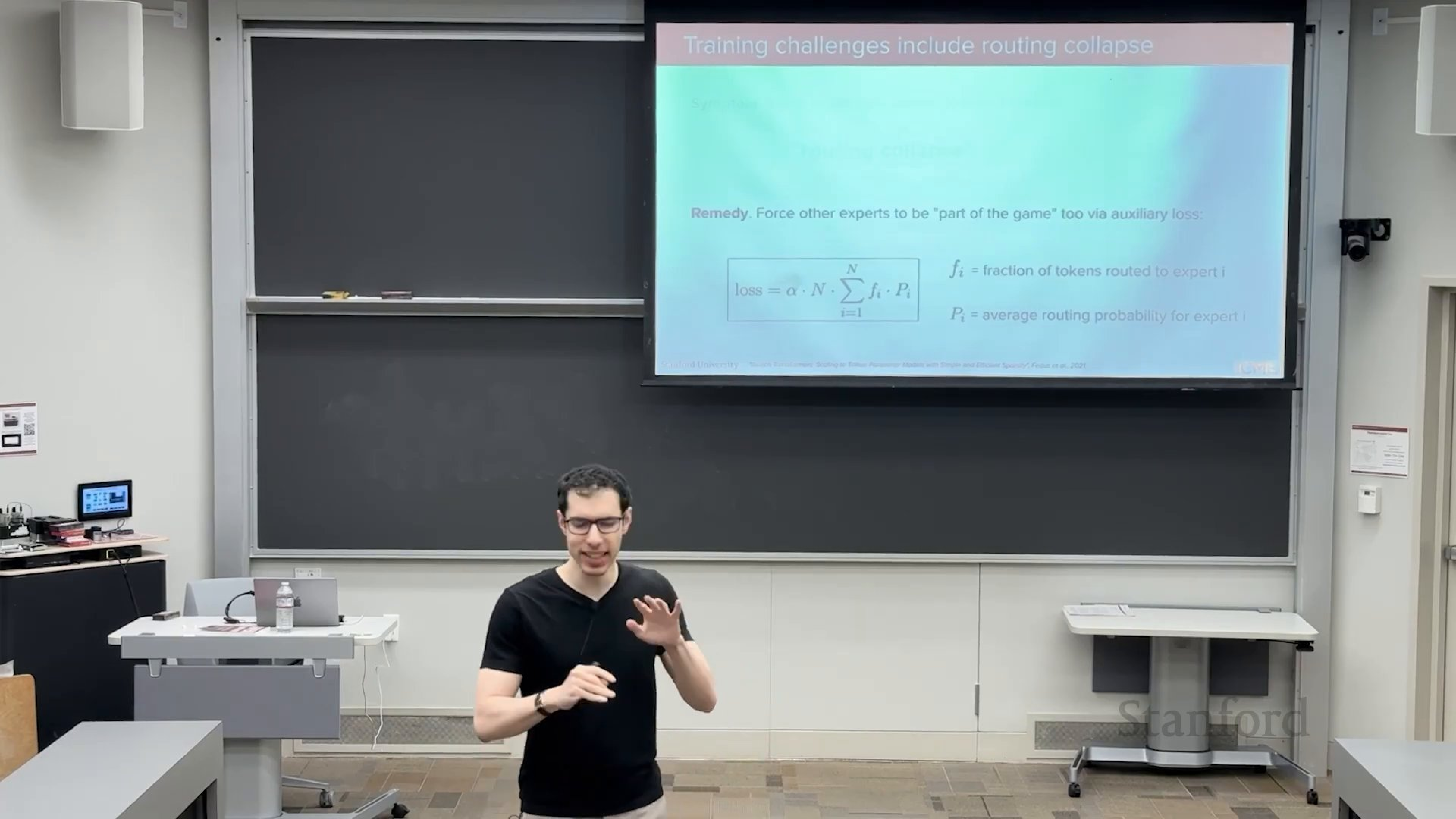
"Switch Transformers: Scaling to Trillion Parameter Models with Simple and Efficient Sparsity", Fedus et al., 2021
Stanford


Training challenges include routing collapse
Remedy. Force other experts to be "part of the game" too via auxiliary loss:
$\boxed{\text{loss} = \alpha \cdot N \cdot \sum_{i=1}^{N} f_i \cdot P_i}$
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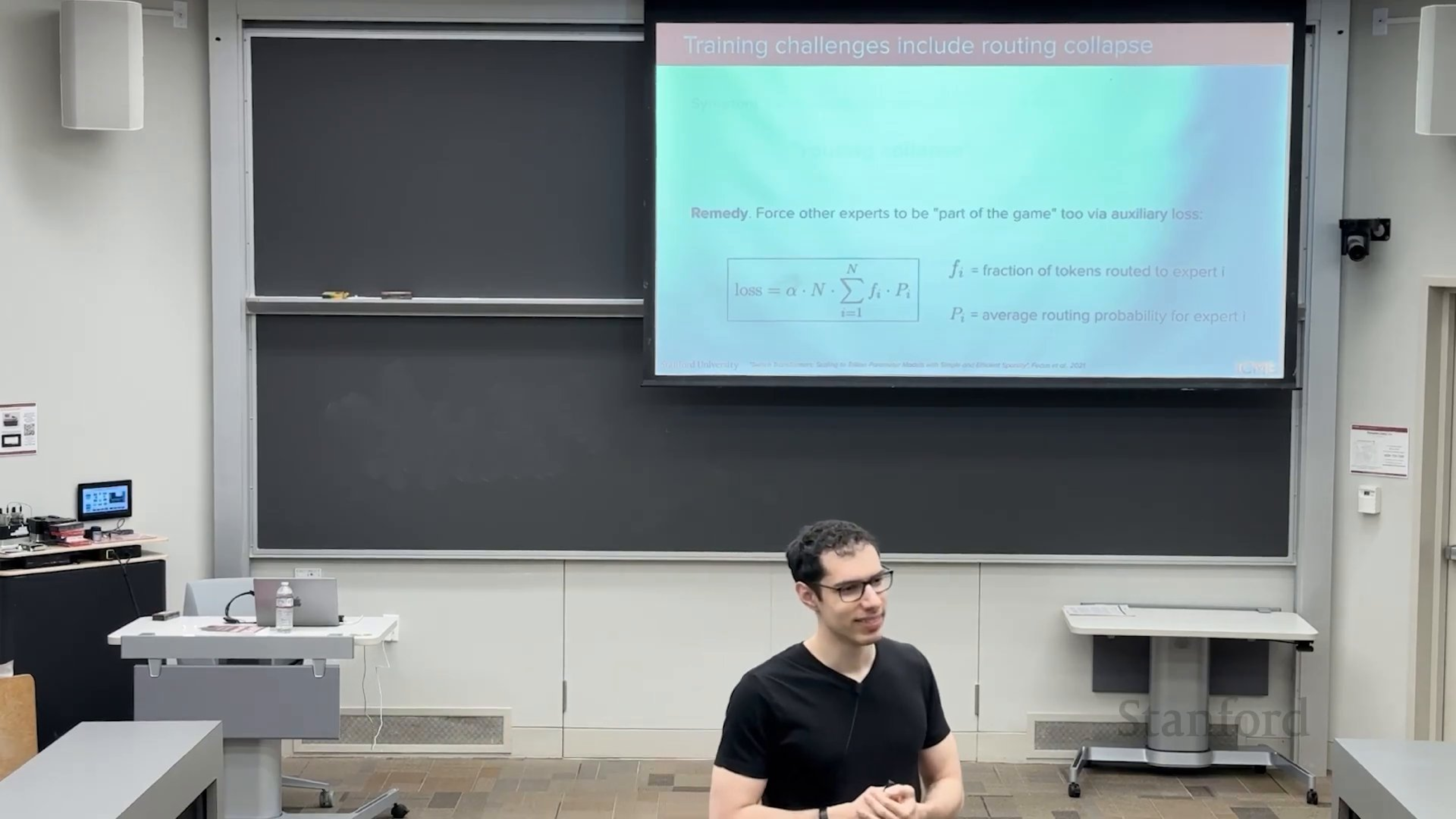
ICME
Stanford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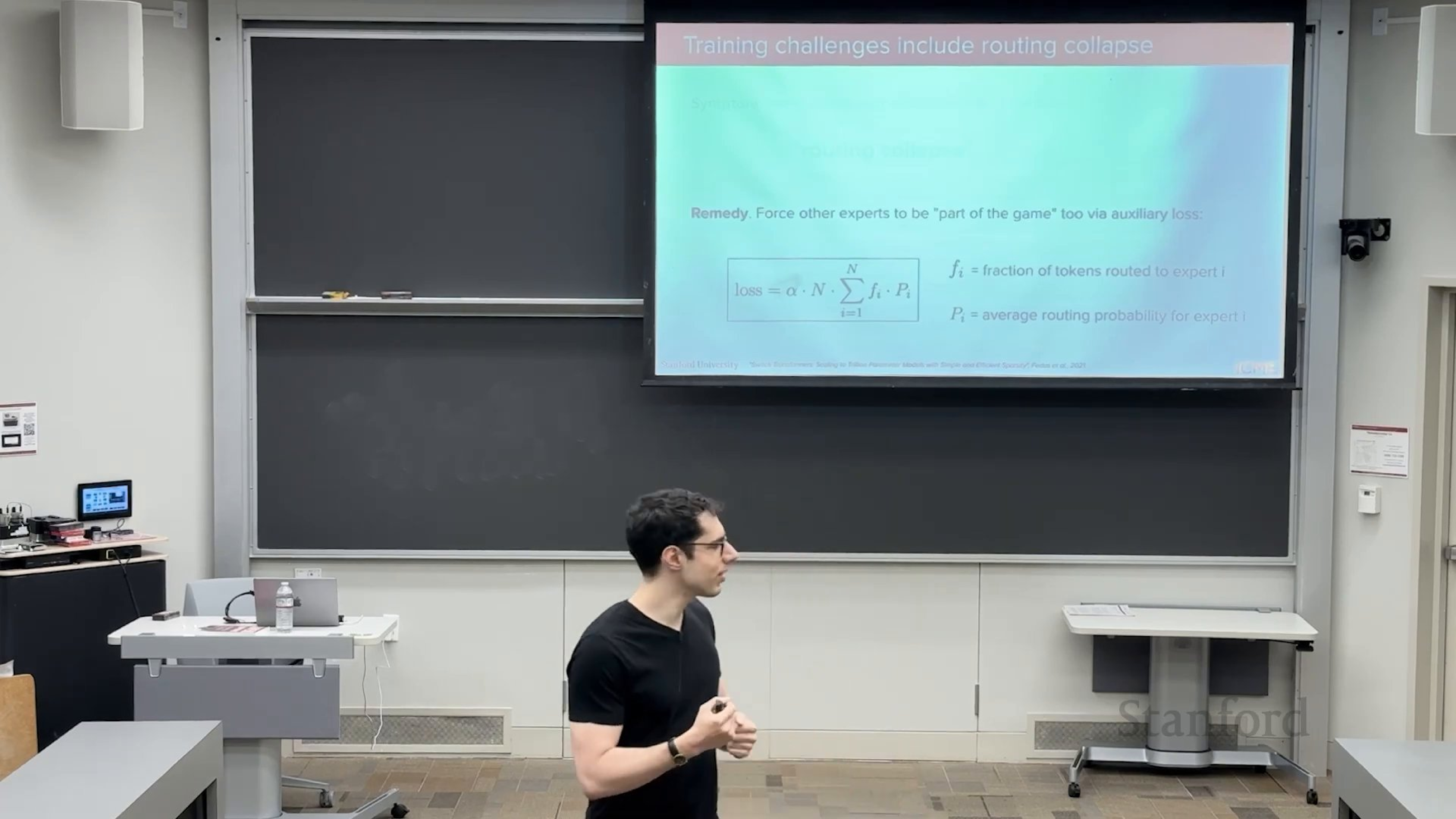
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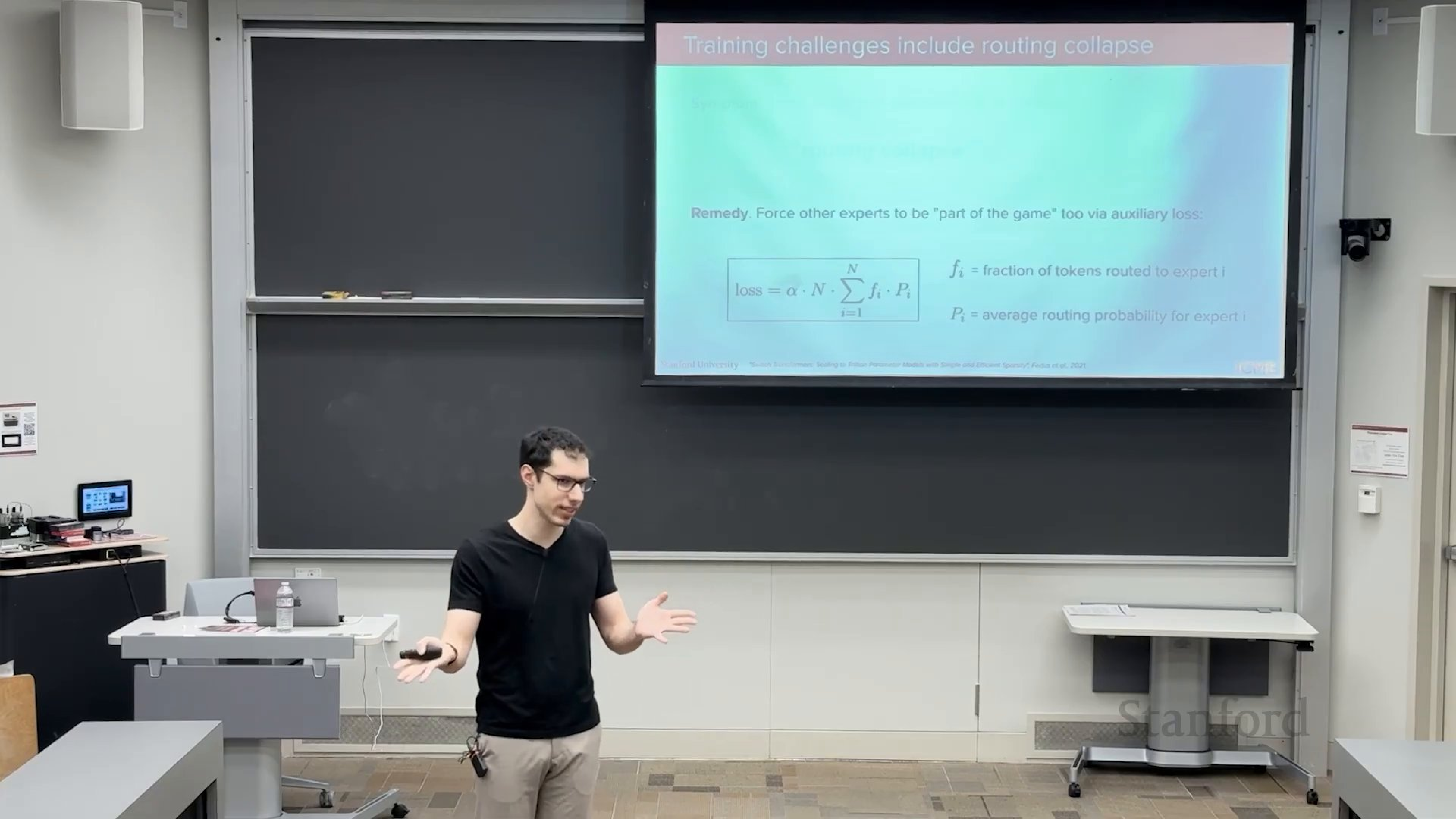
ICME
Stanford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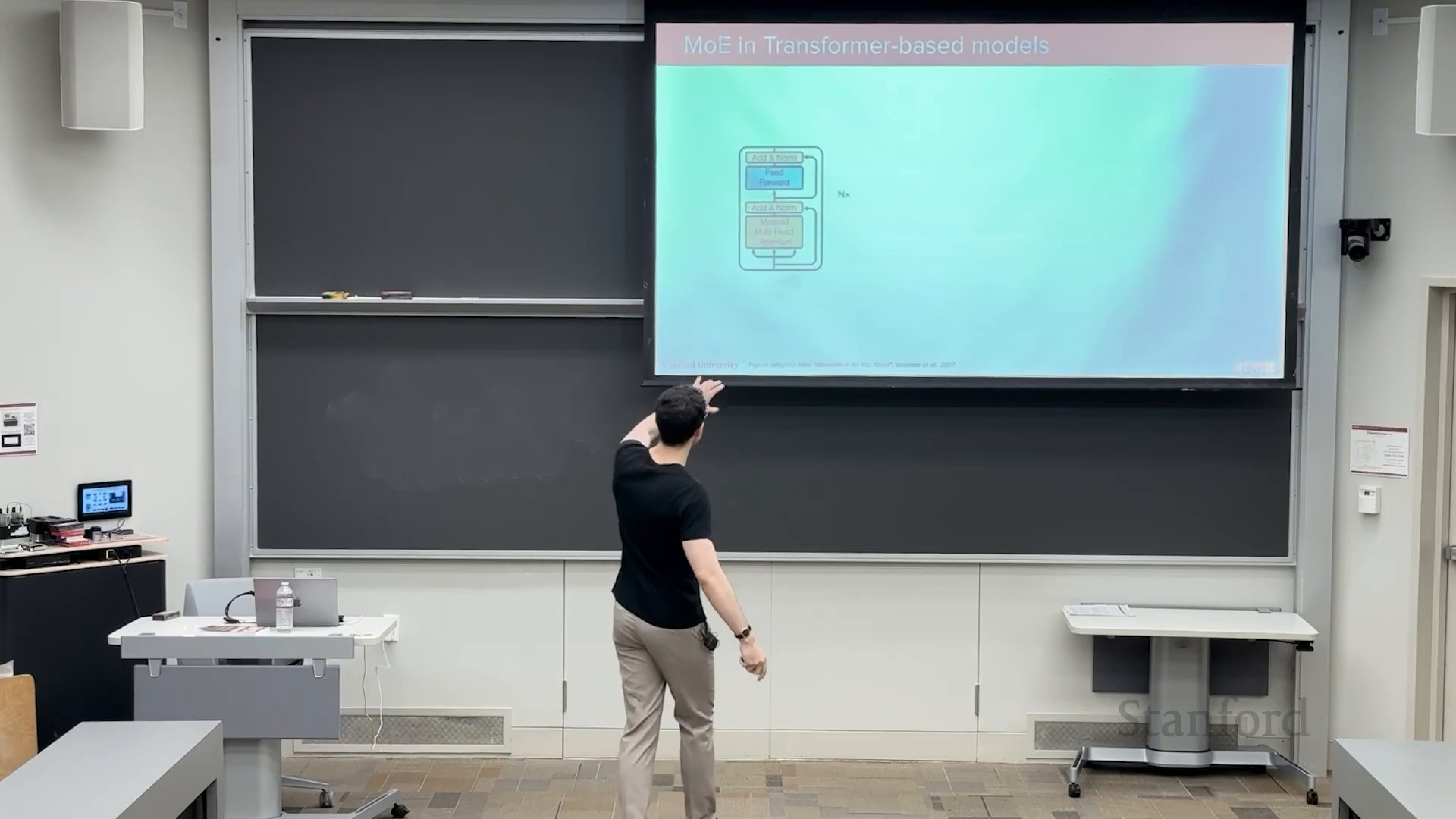
MoE in Transformer-based models
Add & Norm
Feed Forward
Add & Norm
Masked Multi Head Attention
N×
Stanford University
Figure adapted from "Attention is All You Need", Vaswani et al., 2017
Stanford


MoE in Transformer-based models
Add & Norm
Feed Forward
Add & Norm
Masked Multi-Head Attention
N×
Stanford University
Figure adapted from "Attention is All You Need" Vaswani et al. 2017
Stanford


MoE in Transformer-based models
Routing done **for each token**!
Feed Forward
G
X
FFNN
FFNN
FFNN
$\widehat{y}$
Stanford University
Stanford


MoE in Transformer-based models
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Feed Forward
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FFNN
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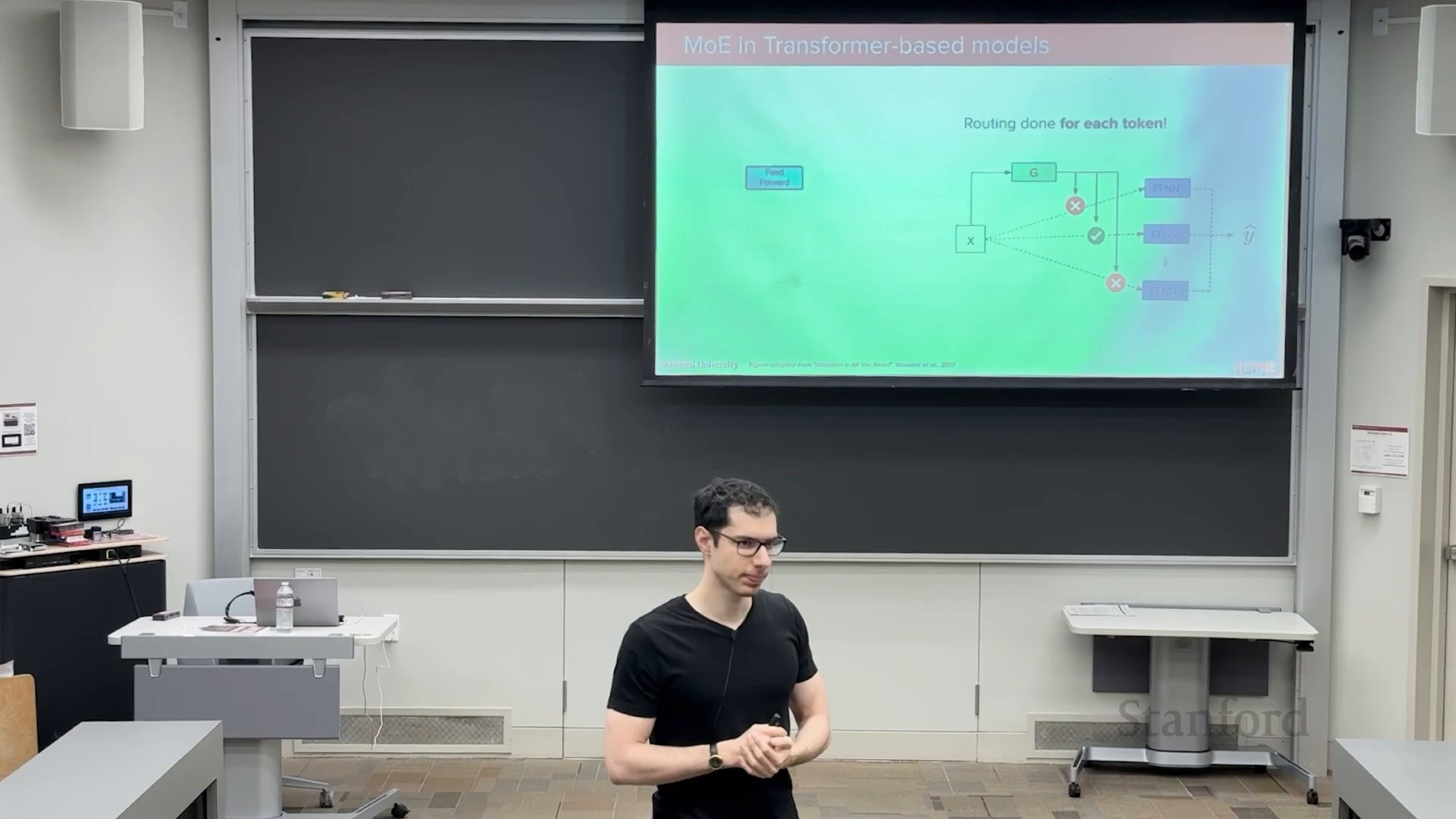
ICME
Stanford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X
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FFNN
$\hat{y}$
Stanford University
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ICME
Stanford


MoE in Transformer-based models
Add & Norm
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Masked Multi-Head Attention
Nx
Stanford University
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Stanford


MoE in Transformer-based models
Add & Norm
Feed Forward
Add & Norm
Masked Multi-Head Attention
N×
Stanford University
Figure adapted from "Attention is All You Need", Vaswani et al., 2017
ICME
Stanford


MoE in Transformer-based models
Add & Norm
Feed Forward
Add & Norm
Masked Multi-Head Attention
N×
Stanford University
Figure adapted from "Attention is All You Need", Vaswani et al., 2017
Stanford

Interpreting experts

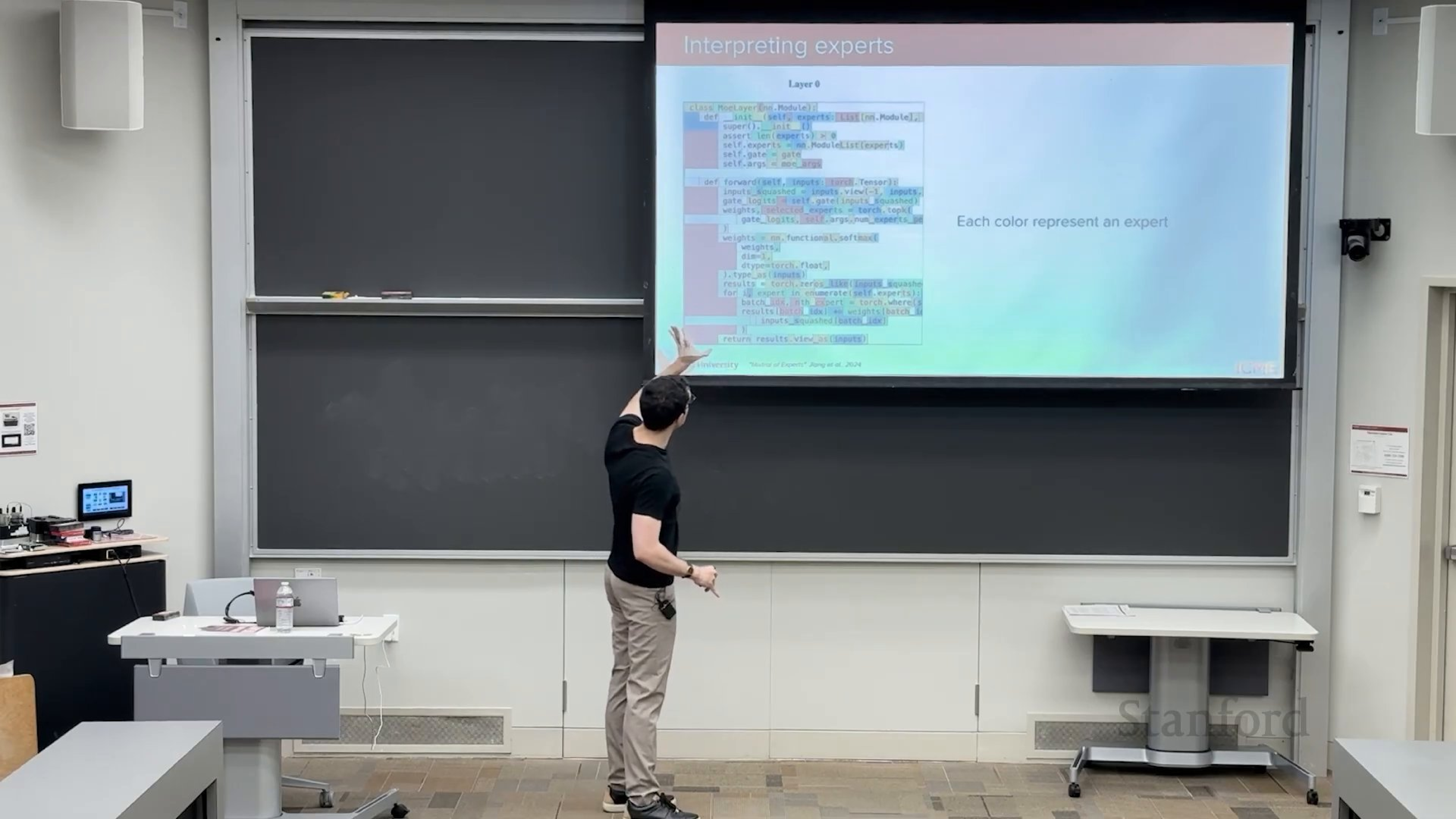
Layer 0

```
class MoeLayer(nn.Module):
    def __init__(self, experts: List[nn.Module],
        super().__init__()
        assert len(experts) > 0
        self.experts = nn.ModuleList(experts)
        self.gate = gate
        self.args = moe_args

    def forward(self, inputs: torch.Tensor):
        inputs_squashed = inputs.view(-1, inputs.
        gate_logits = self.gate(inputs_squashed)
        weights, selected_experts = torch.topk(
            gate_logits, self.args.num_experts_pe
        )
        weights = nn.functional.softmax(
            weights,
            dim=1,
            dtype=torch.float,
        ).type_as(inputs)
        results = torch.zeros_like(inputs_squashe
        for i, expert in enumerate(self.experts):
            batch_idx, nth_expert = torch.where(s
            results[batch_idx] += weights[batch_ic
                inputs_squashed[batch_idx]
            )
        return results.view_as(inputs)
```

Each color represent an expert

Stanford



Interpreting experts
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Each color represent an expert
"Mixtral of Experts" Jiang et al. 2024
Stanford


Transformers & Large Language Models
LLM overview
MoE-based LLMs
Response generation
Prompting strategies
Inference optimizations
ICME
Stanford


Transformers &
Large Language
Models
LLM overview
MoE-based LLMs
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ICME
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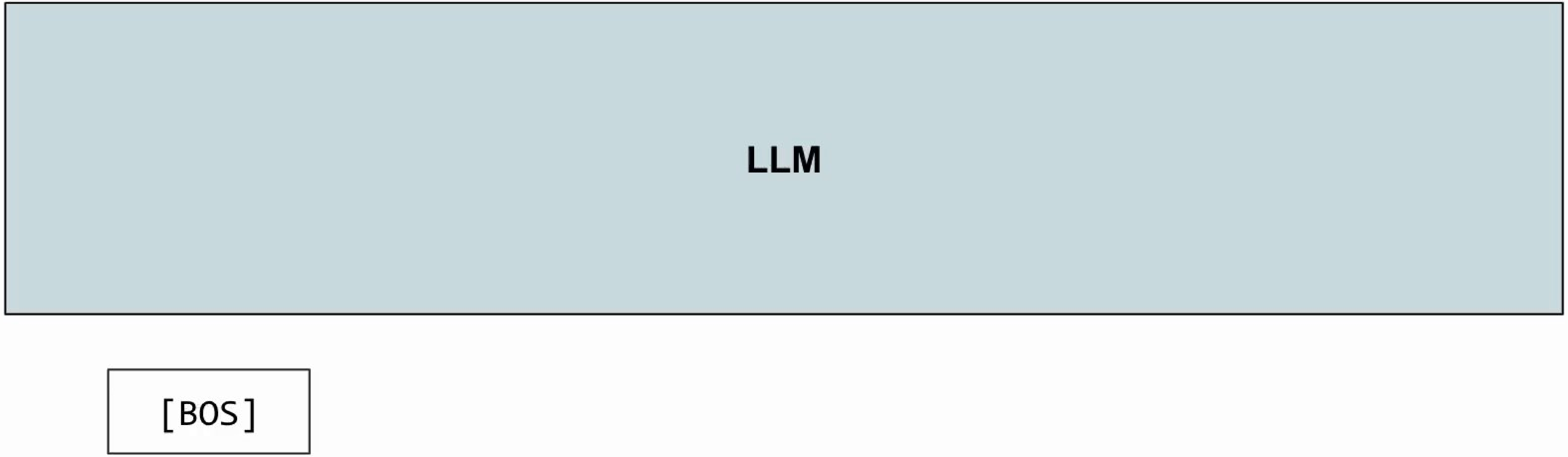
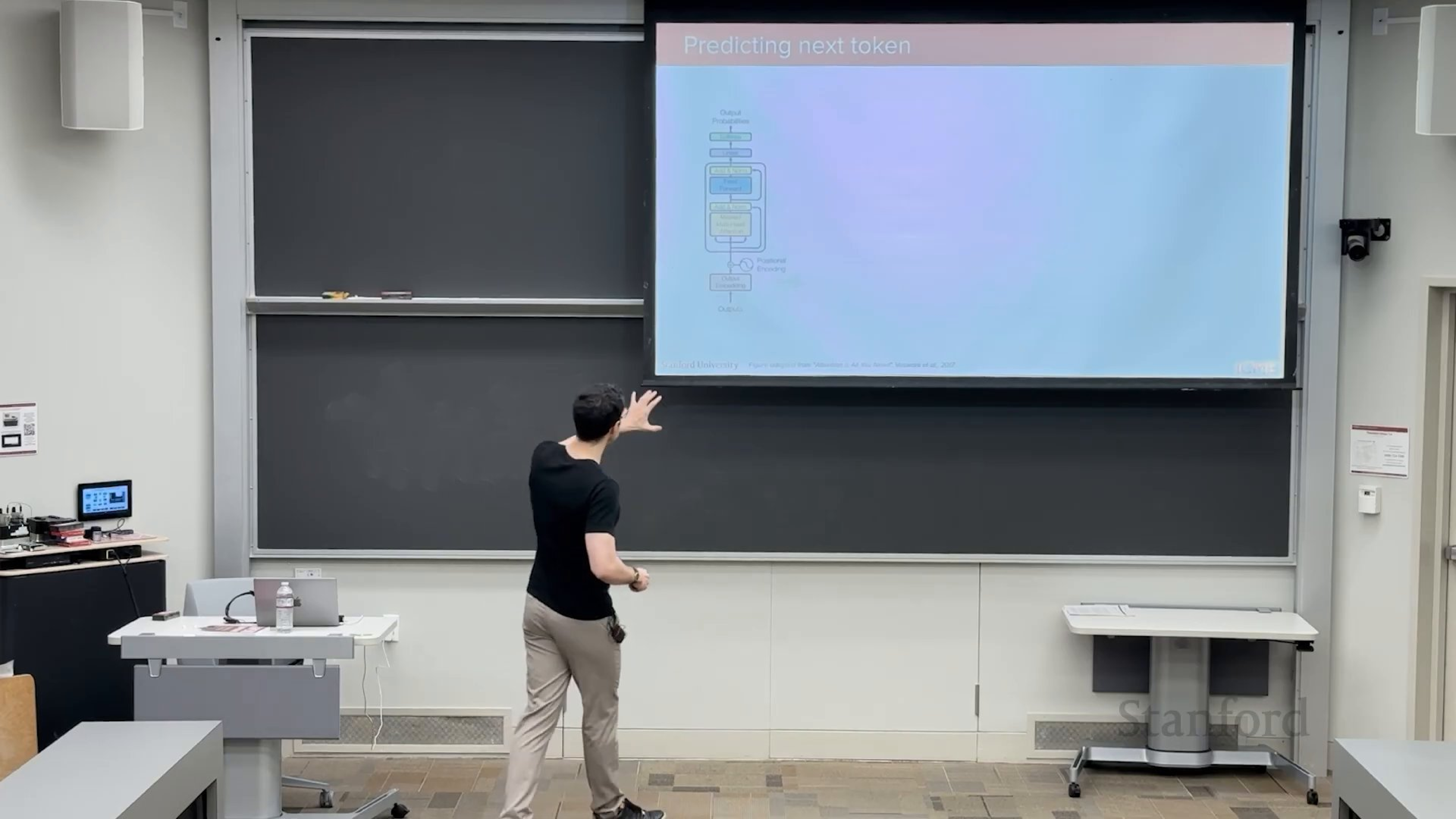
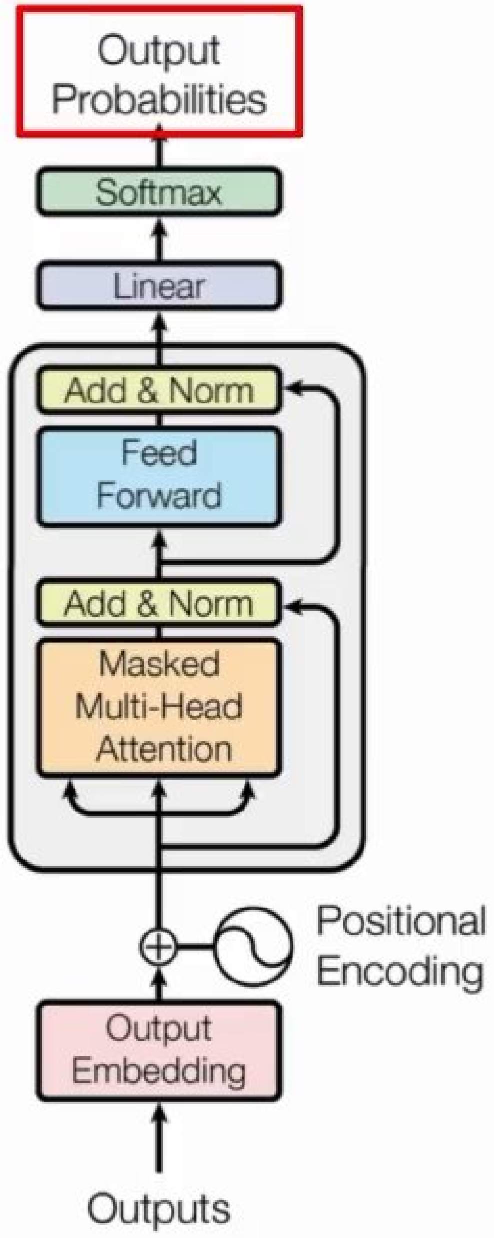
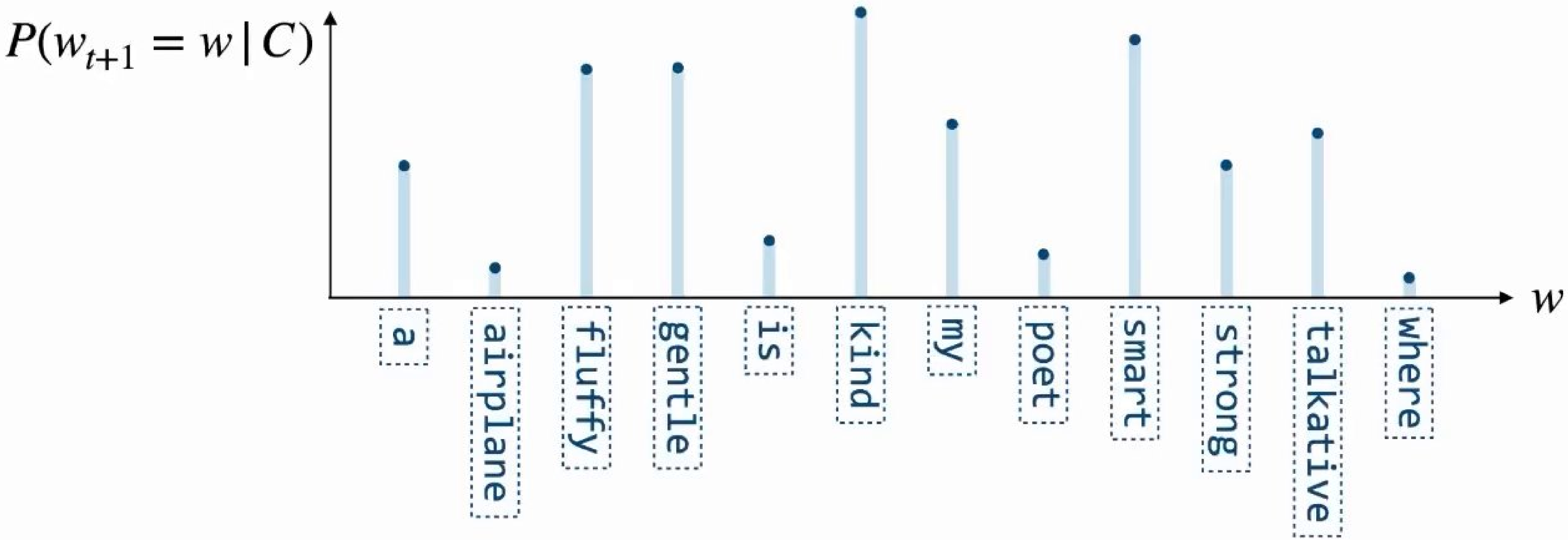
Next token prediction




Predicting next token
Output Probabilities
Add & Norm
Feed Forward
Add & Norm
Positional Encoding
Output Embedding
Stanford University
Stanford

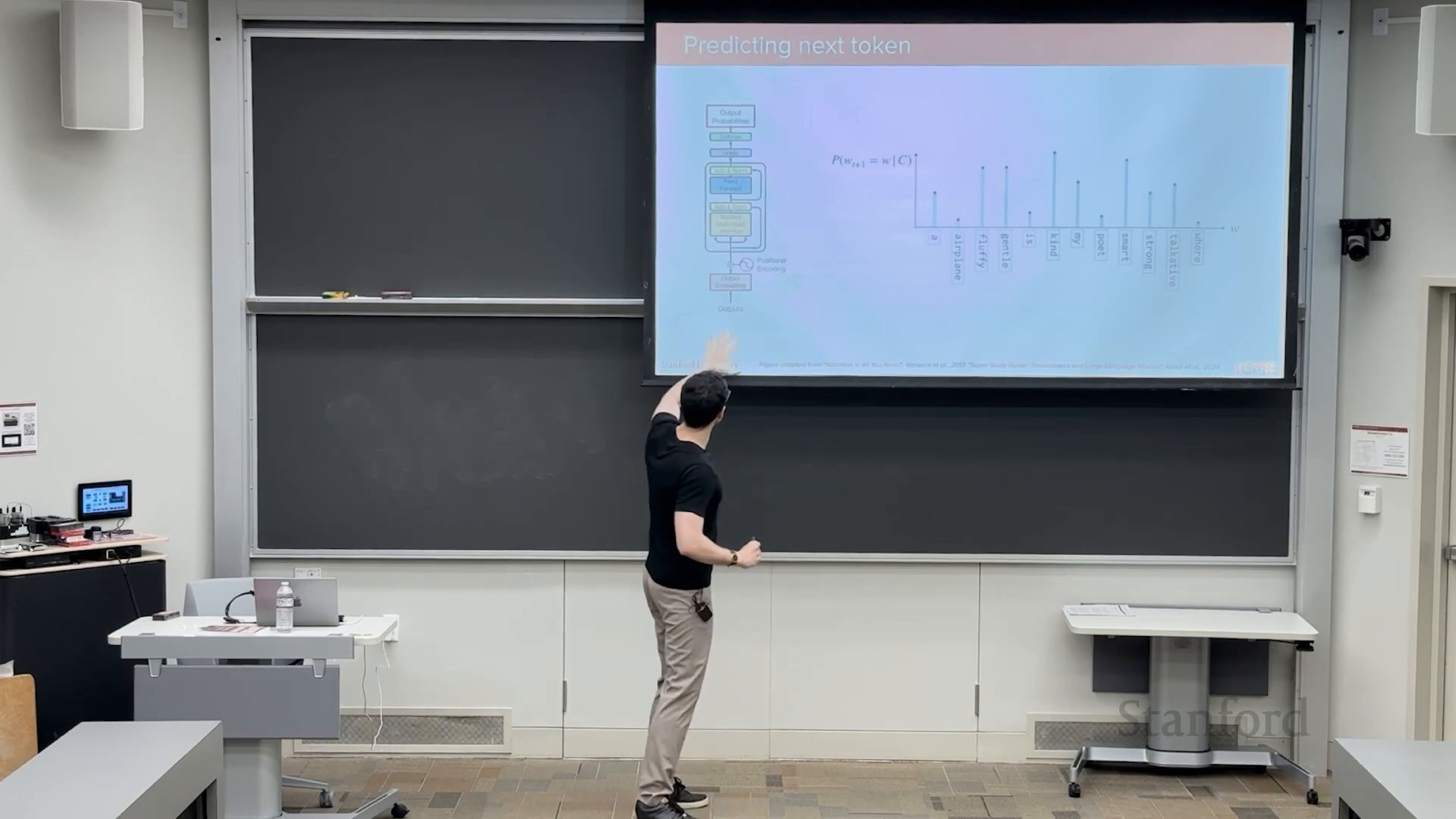
Predicting next token



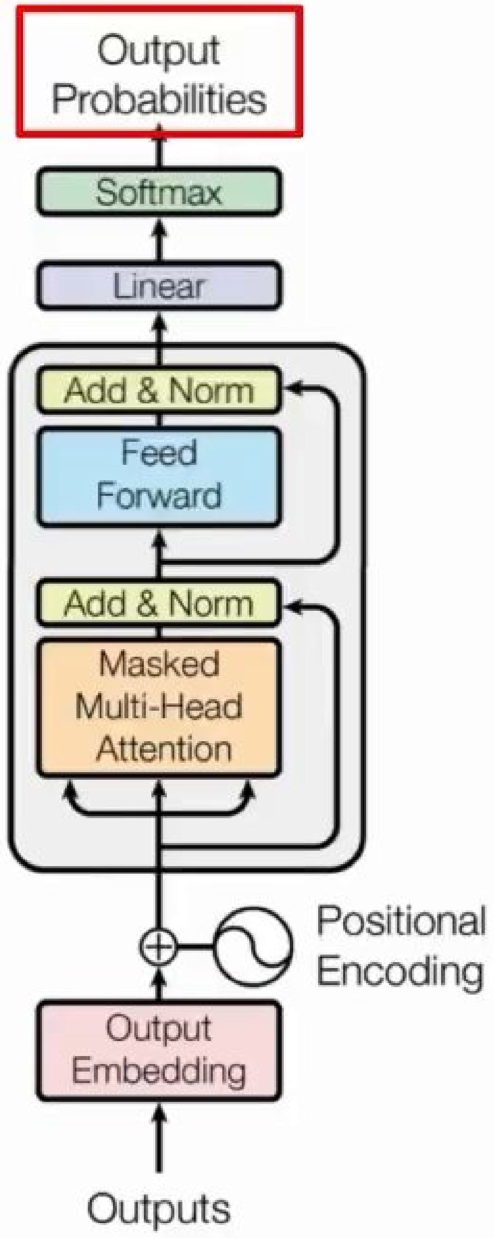


Stanford

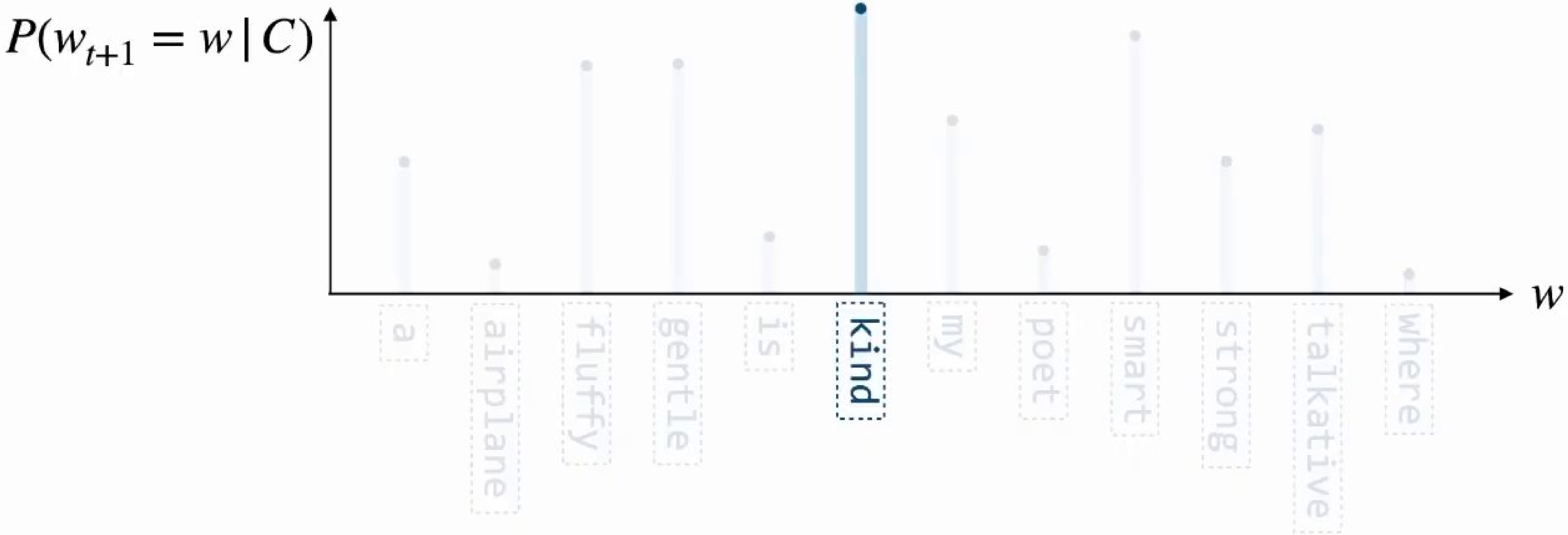
Figure adapted from "Attention is All You Need", Vaswani et al., 2017. "Super Study Guide: Transformers and Large Language Models", Amidi et al., 2024.


Predicting next token
Output Probabilities
Positional Encoding
Outputs
$P(w_{t+1} = w \mid C)$
w
a
airplane
fluffy
gentle
is
kind
my
poet
smart
strong
talkative
where
Stanford

Predicting next token with greedy decodi



1st idea. Take token with highest predicted probability



Stanford

Figure adapted from "Attention is All You Need", Vaswani et al., 2017. "Super Study Guide: Transformers and Large Language Models", Amidi et al., 2024.

Predicting next token with greedy decoding
1st idea. Take token with highest predicted probability
$P(w_{t+1} = w \mid C)$
w
k1nd
Positional Encoding
Outputs
Limitations. Output not optimal, natural and/or diverse
Stanford University
Stanford


Predicting next token with greedy decoding
1st idea. Take token with highest predicted probability
Output Probabilities
Positional Encoding
Output Embedding
Outputs
$P(w_{t+1} = w \mid C)$
w
kind
Limitations. Output not optimal, natural and/or diverse
Stanford University
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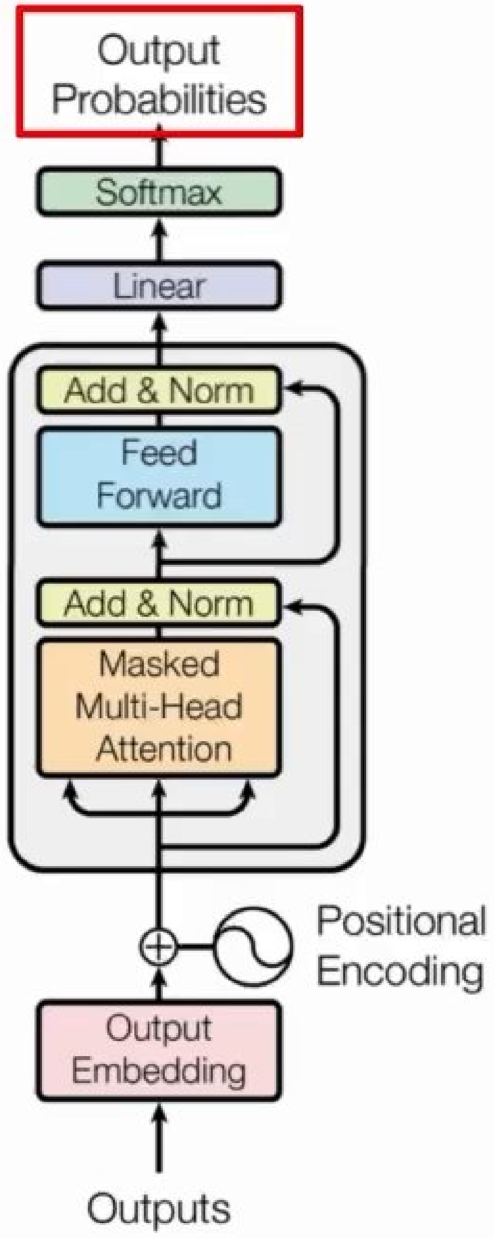
Predicting next token with beam search



2nd idea. Keep k paths that are the most likely

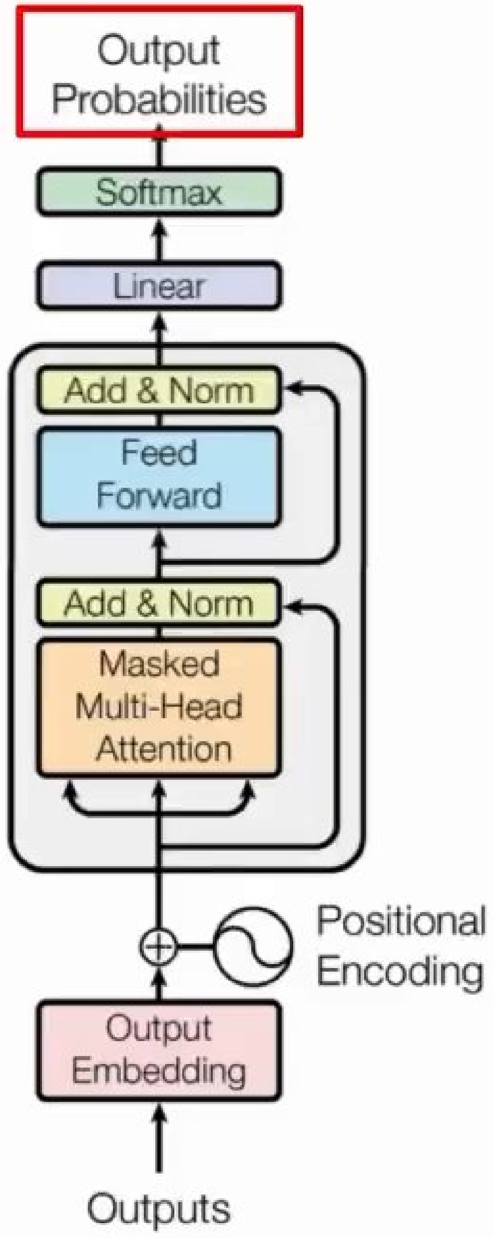
[BOS]

Stanford

Figure adapted from "Attention is All You Need", Vaswani et al., 2017.

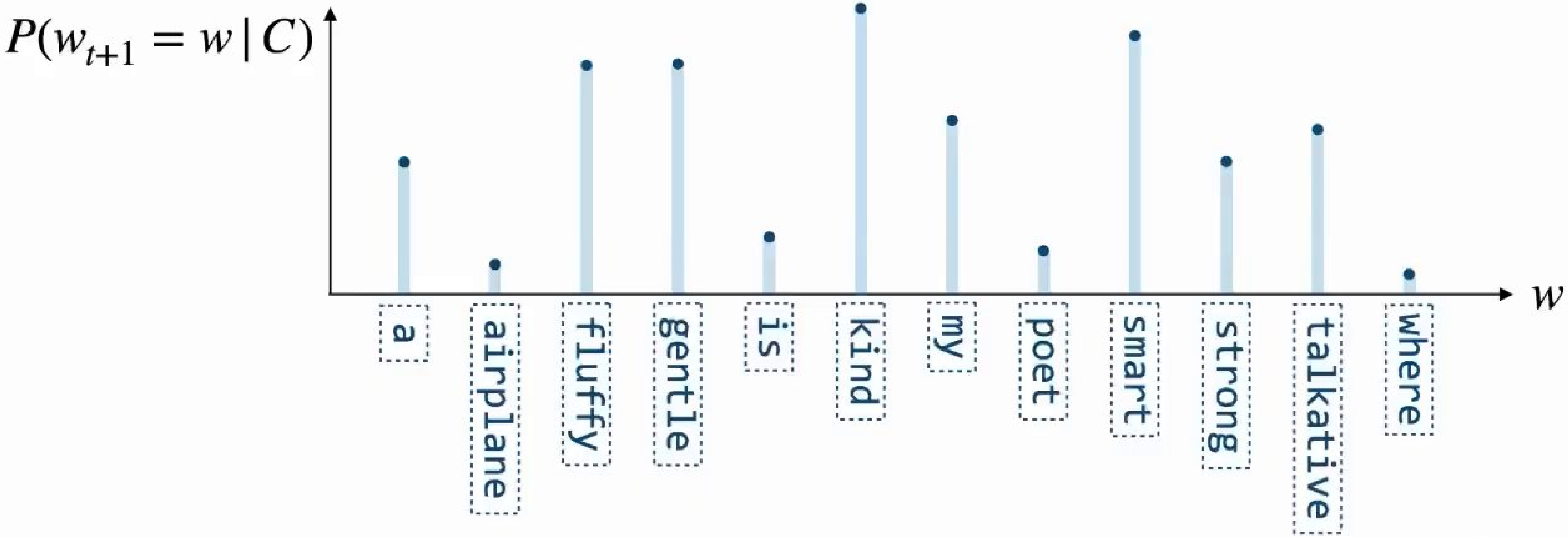
Predicting next token with beam search
2nd idea. Keep k paths that are the most likely
Output Probabilities
Positional Encoding
Outputs
[BOS]
a
cute
teddy
bear
Ends at [EOS]
Stanford University
Stanford

Predicting next token with sampling



3rd idea. Sample next token from probability distribution:

$$\boxed{\widehat{w}_{t+1} \sim P(w_{t+1}|C)}$$



"Super Study Guide: Transformers and Large Language Models", Amidi et al., 2024.

Predicting next token with sampling
3rd idea. Sample next token from probability distribution:
$\widehat{w}_{t+1} \sim P(w_{t+1}|C)$
$P(w_{t+1} = w \mid C)$
w
a
airplane
fluffy
gentle
is
kind
my
poet
smart
strong
talkative
where
Output Probabilities
Positional Encoding
Output Embedding
Outputs
Stanford University
"Super Study Guide: Transformers and Large Language Models", Amidi et al., 2024
Stanford

Predicting next token with sampling
3rd idea. Sample next token from probability distribution:
$\boxed{\widehat{w}_{t+1} \sim P(w_{t+1}|C)}$
Output Probabilities
Softmax
Linear
Add & Norm
Feed Forward
Add & Norm
Masked Multi-Head Attention
Positional Encoding
Output Embedding
Outputs
$P(w_{t+1} = w\,|\,C)$
a
airplane
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Stanford University
"Super Study Guide: Transformers and Large Language Models", Amidi et al., 2024
ICME
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Stanford University
"Super Study Guide: Transformers and Large Language Models", Amidi et al., 2024
Stanford


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Stanford University
"Super Study Guide: Transformers and Large Language Models", Amidi et al., 2024
Stanford


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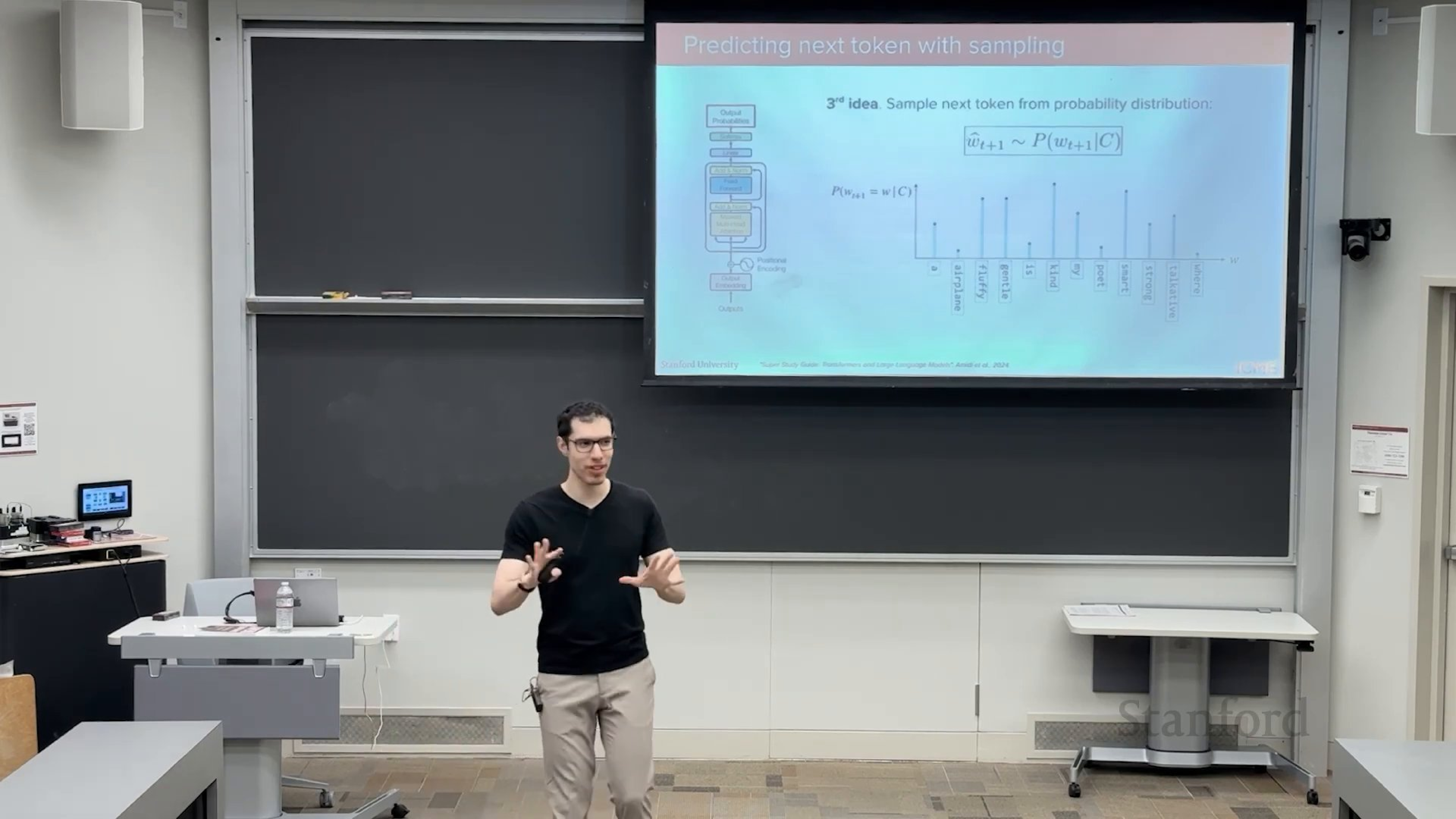
Stanford University
"Super Study Guide: Transformers and Large Language Models", Amidi et al., 2024
Stanford



Predicting next token with sampling
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Output Probabilities
Positional Encoding
Output Embedding
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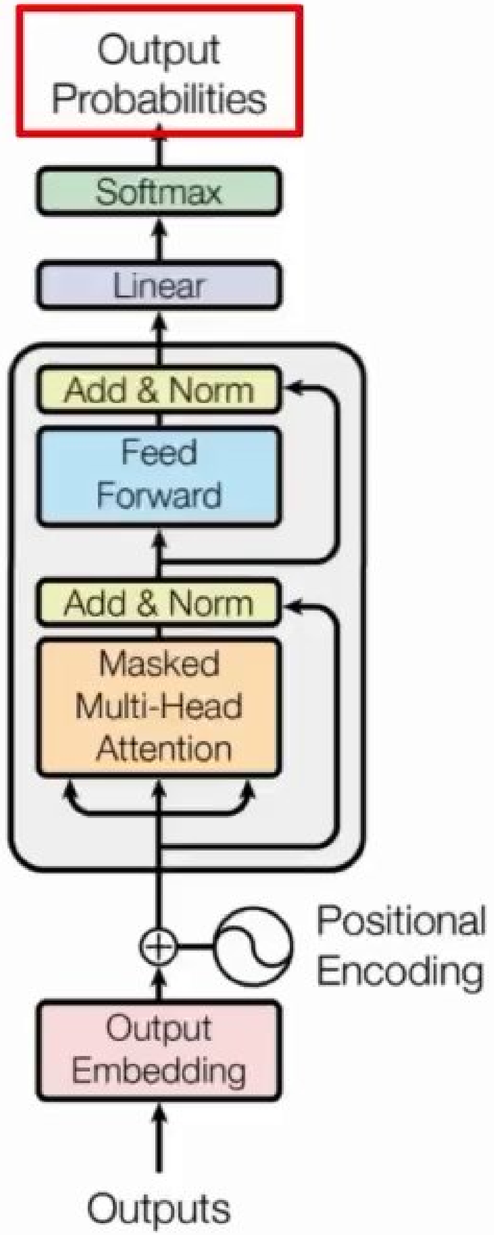
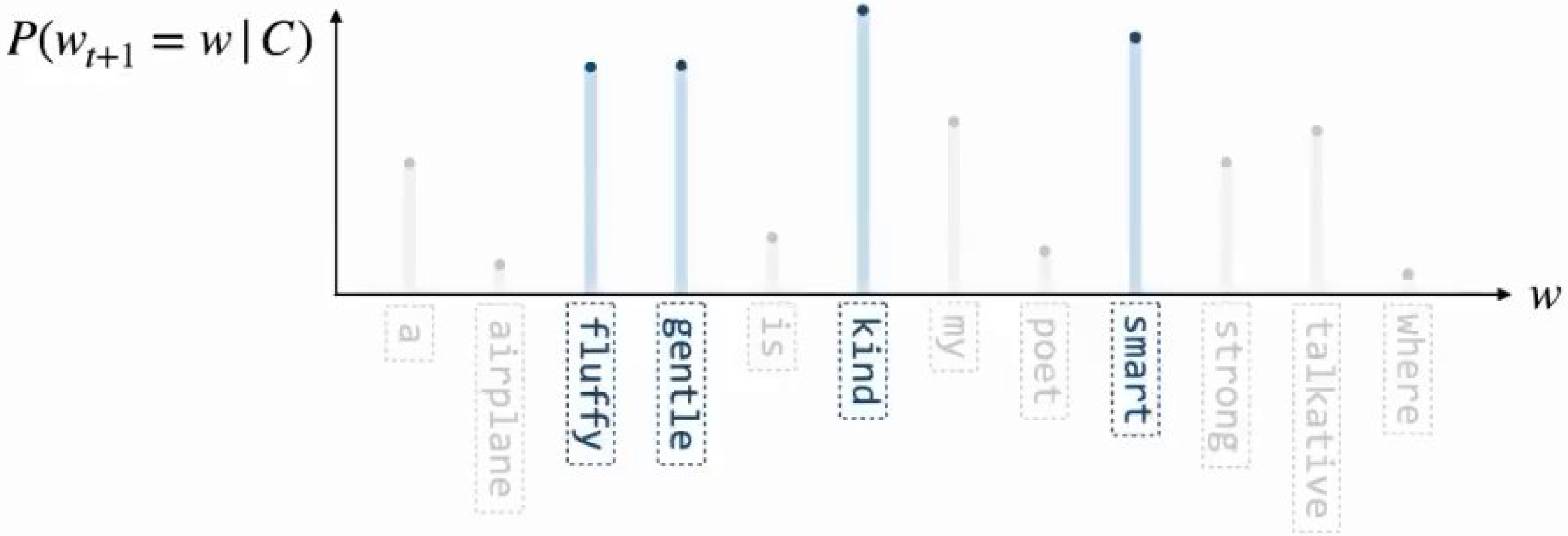
w
Stanford University
"Super Study Guide: Transformers and Large Language Models", Amidi et al., 2024
ICME
Stanford

Sampling strategies



- **Top-k**: Sample among top k most probable tokens

k = 4

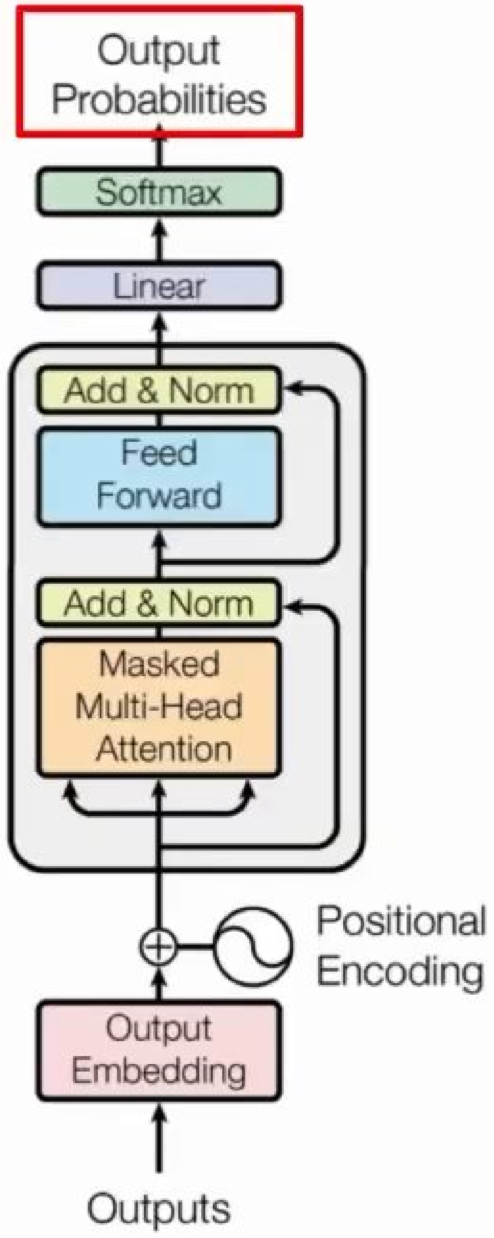


Stanford

Next token prediction

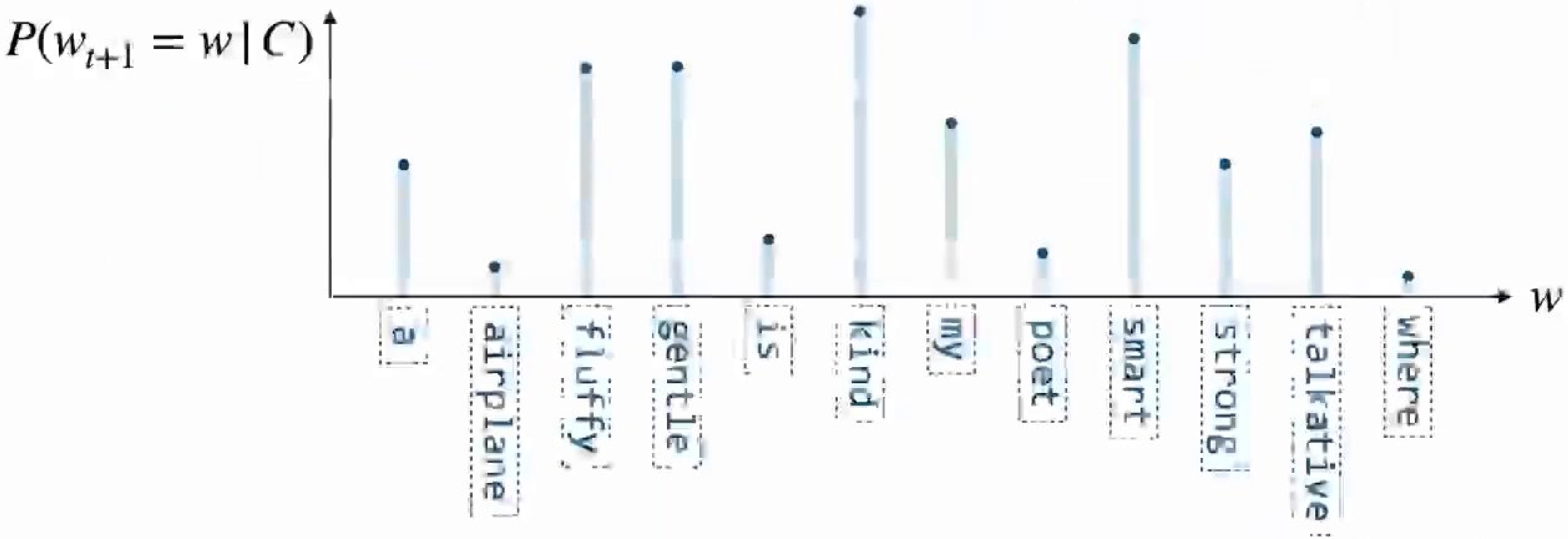
But **how** are probabilities **obtained**?

Predicting next token with sampling



3rd idea. Sample next token from probability distribution:

$$\boxed{\widehat{w}_{t+1} \sim P(w_{t+1}|C)}$$



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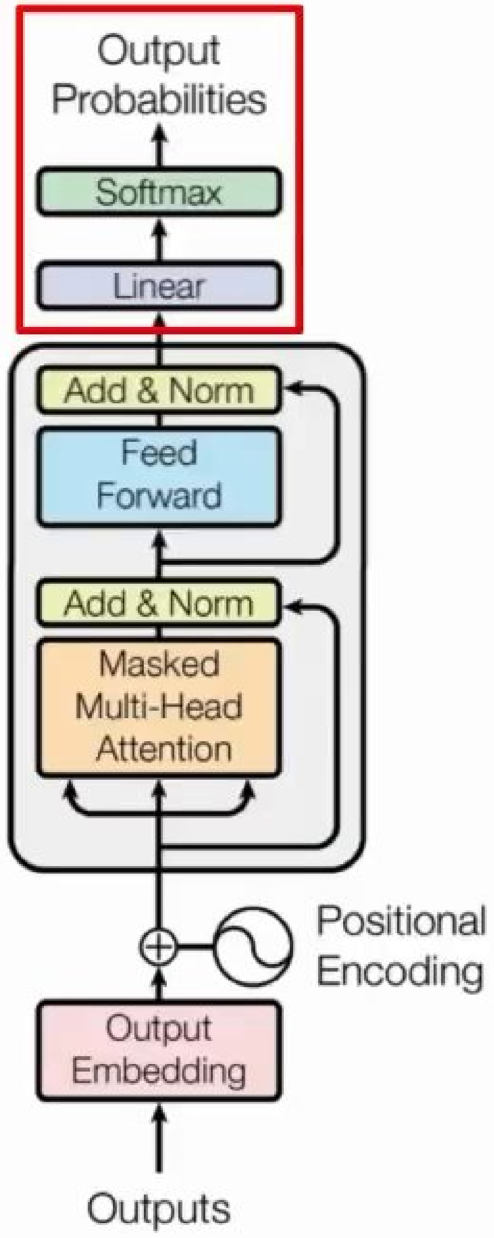
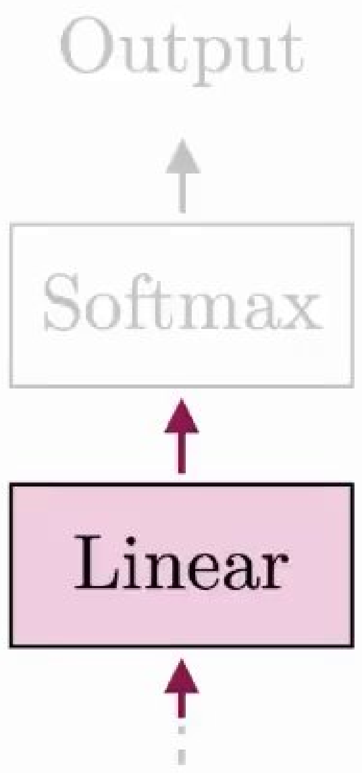
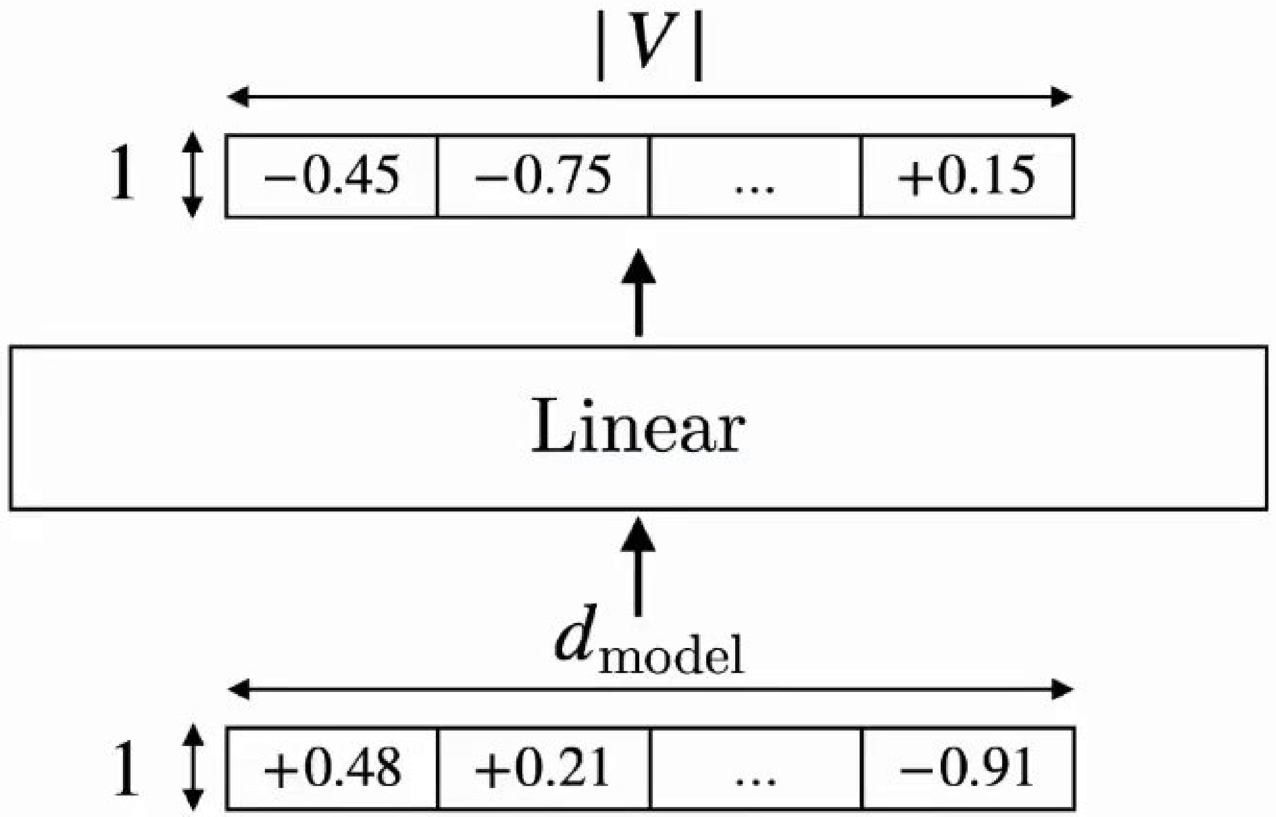
Probability computation







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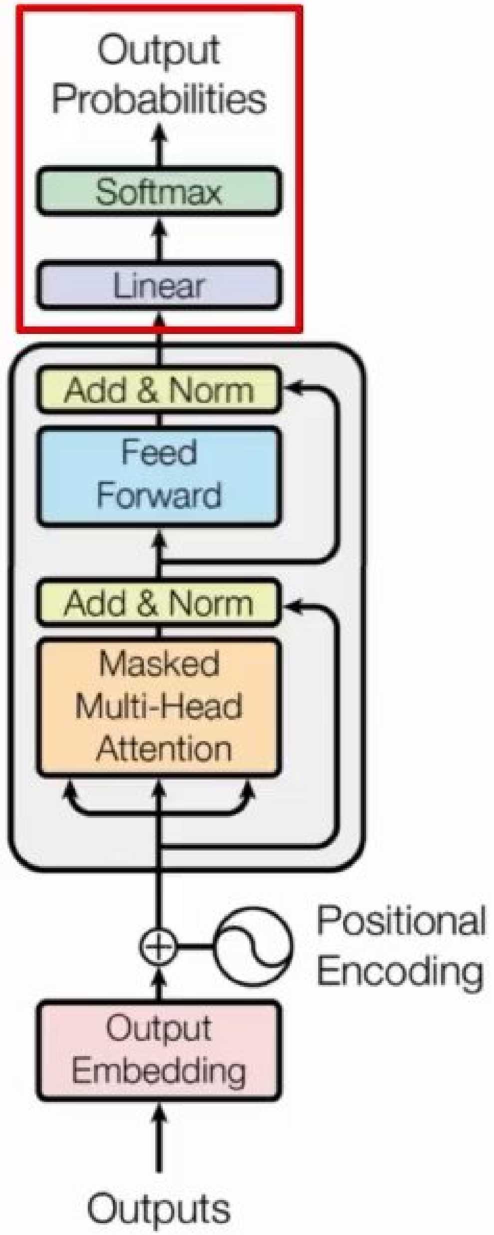
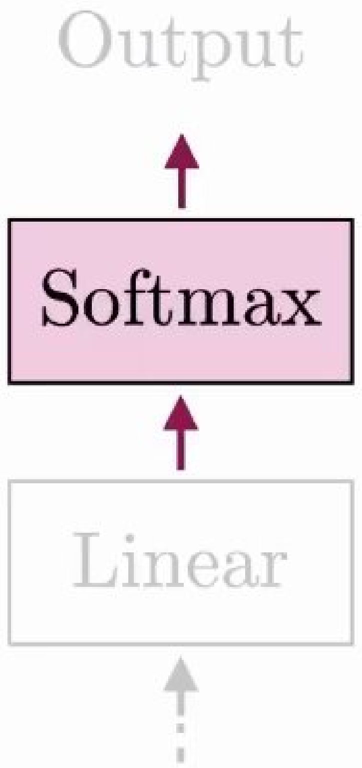
Probability computation
Output Probabilities
Positional Encoding
Outputs
Linear
|V|
1
−0.45
−0.75
...
+0.15
Linear
d_model
1
+0.48
+0.21
...
−0.91
Stanford

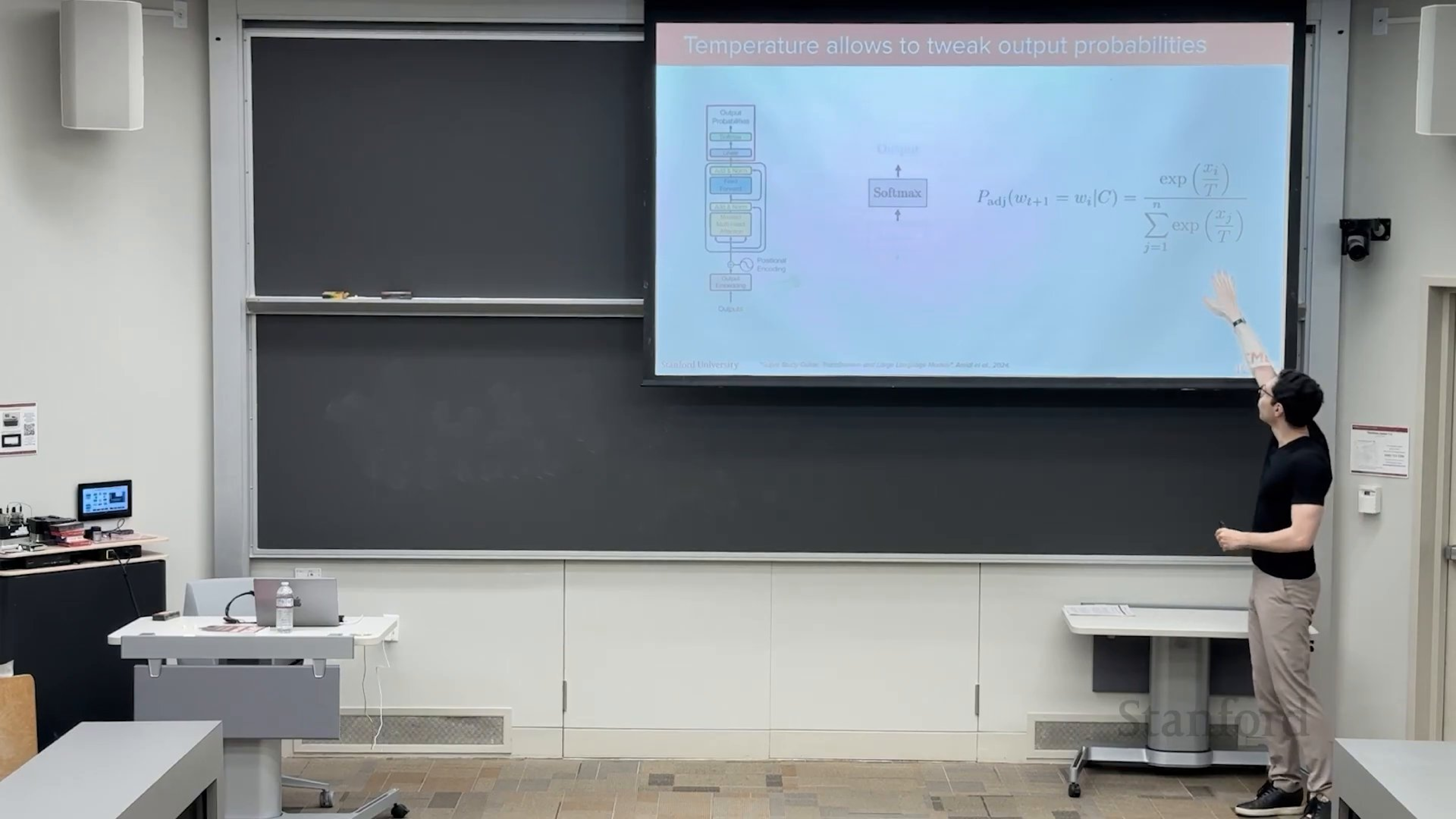
Temperature allows to tweak output prob



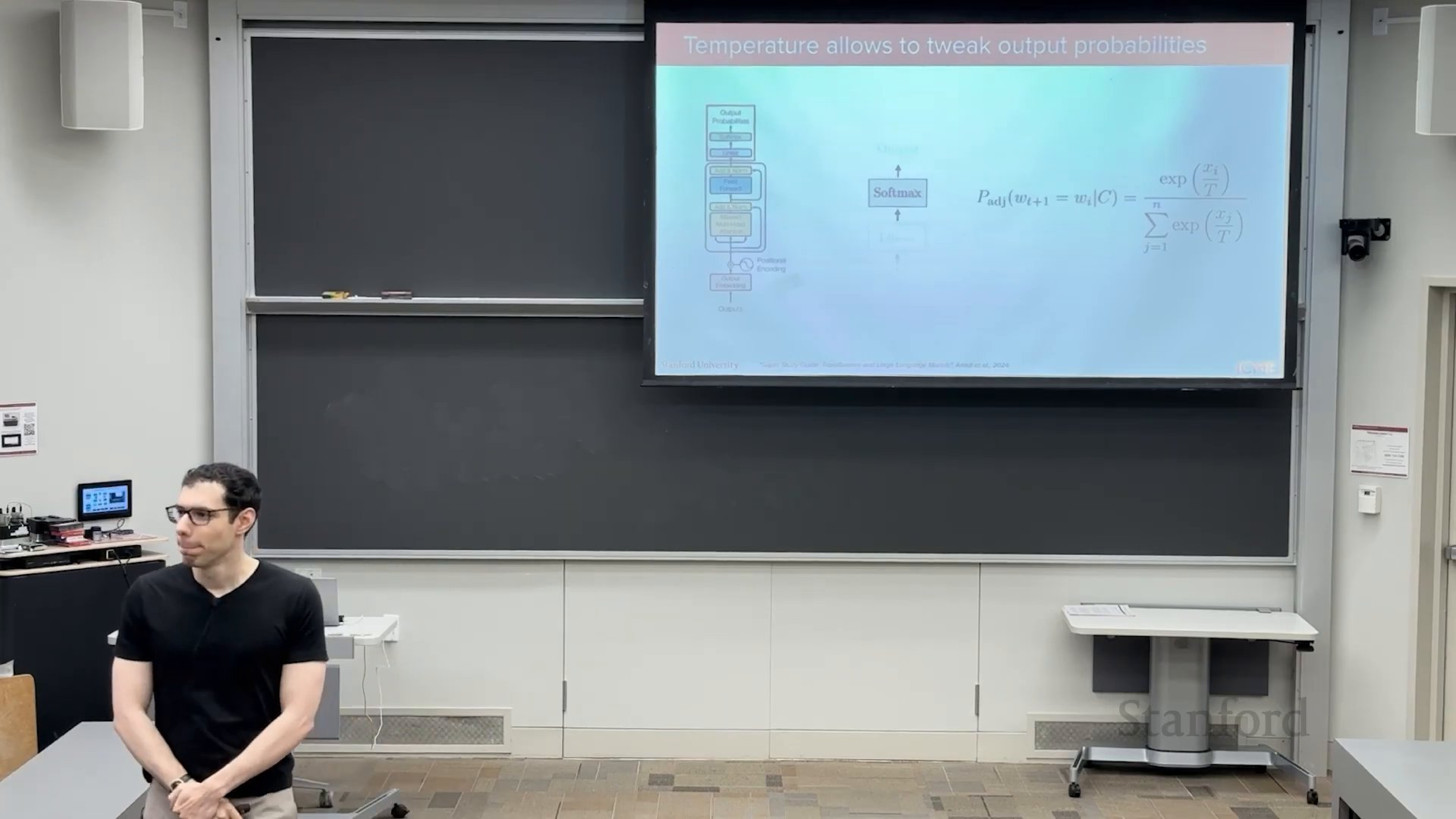


$$P_{\text{adj}}(w_{t+1} = w_i | C) = \frac{\exp\left(\frac{x_i}{T}\right)}{\sum_{j=1}^{n} \exp\left(\frac{x_j}{T}\right)}$$

Stanford



Temperature allows to tweak output probabilities
Output Probabilities
Positional Encoding
Output Embedding
Outputs
Softmax
$$P_{\mathrm{adj}}(w_{t+1} = w_i | C) = \frac{\exp\left(\frac{x_i}{T}\right)}{\sum_{j=1}^{n} \exp\left(\frac{x_j}{T}\right)}$$
Stanford University
Stanford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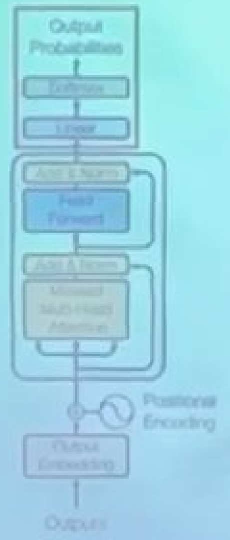
Stanford University
Amidi et al., 2024
Stanford

Temperature allows to tweak output probabilities



Softmax

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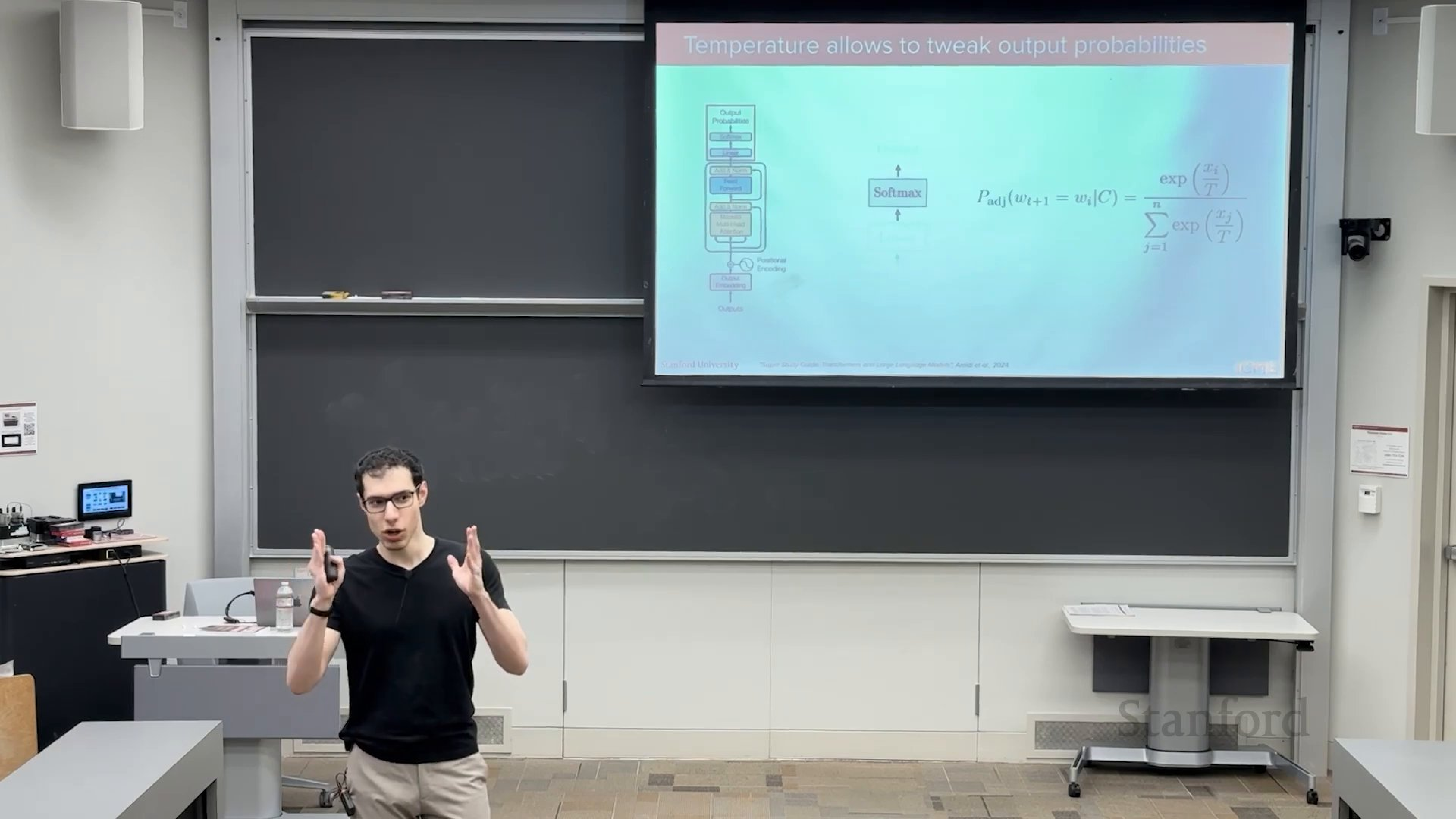
Temperature allows to tweak output probabilities
Output Probabilities
Softmax
Linear
Add & Norm
Feed Forward
Add & Norm
Masked Multi-Head Attention
Positional Encoding
Output Embedding
Outputs
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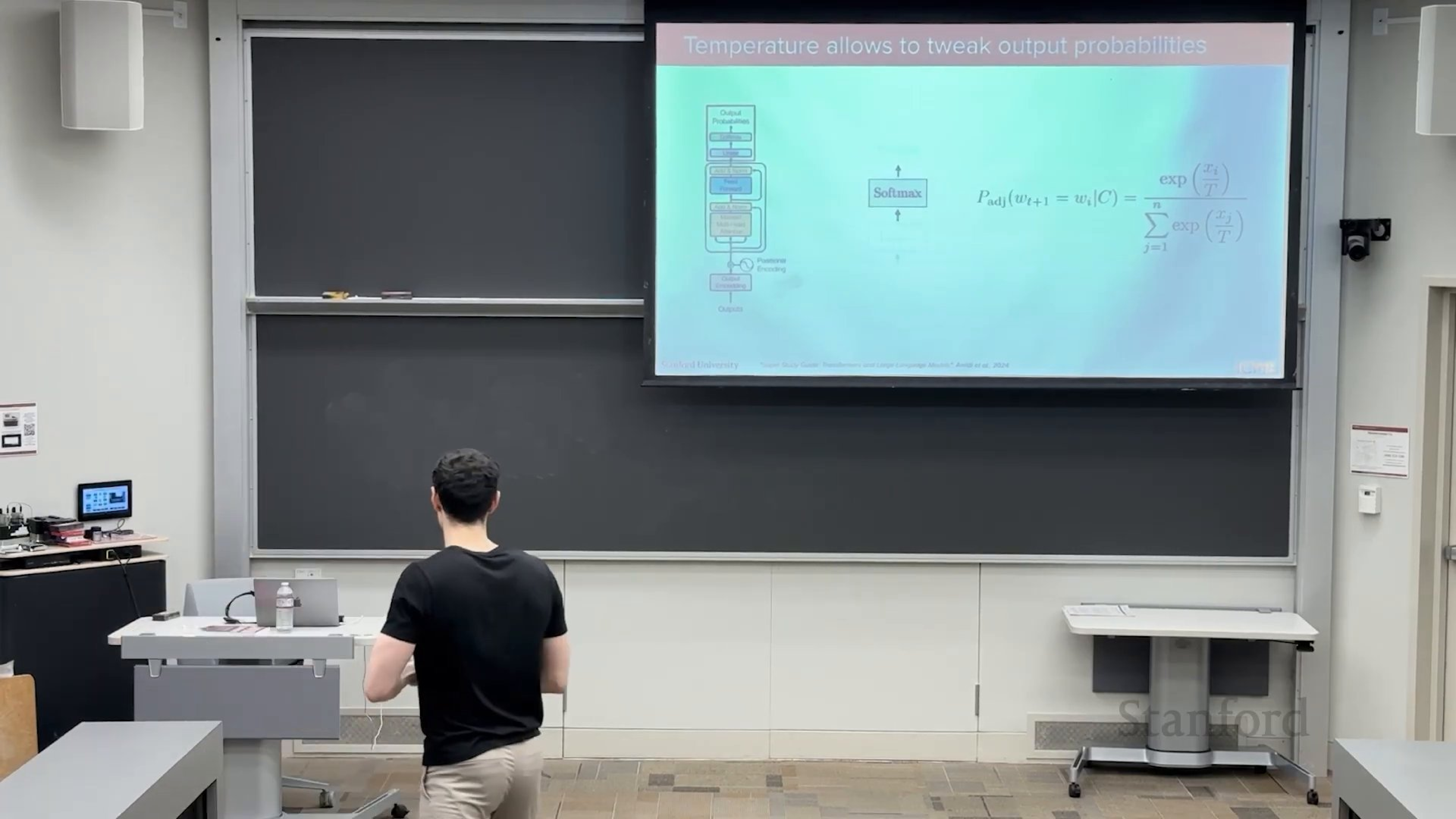
Stanford University
Amidi et al., 2024
Stanford


Temperature allows to tweak output probabilities
Output Probabilities
Positional Encoding
Output Embedding
Outputs
Softmax
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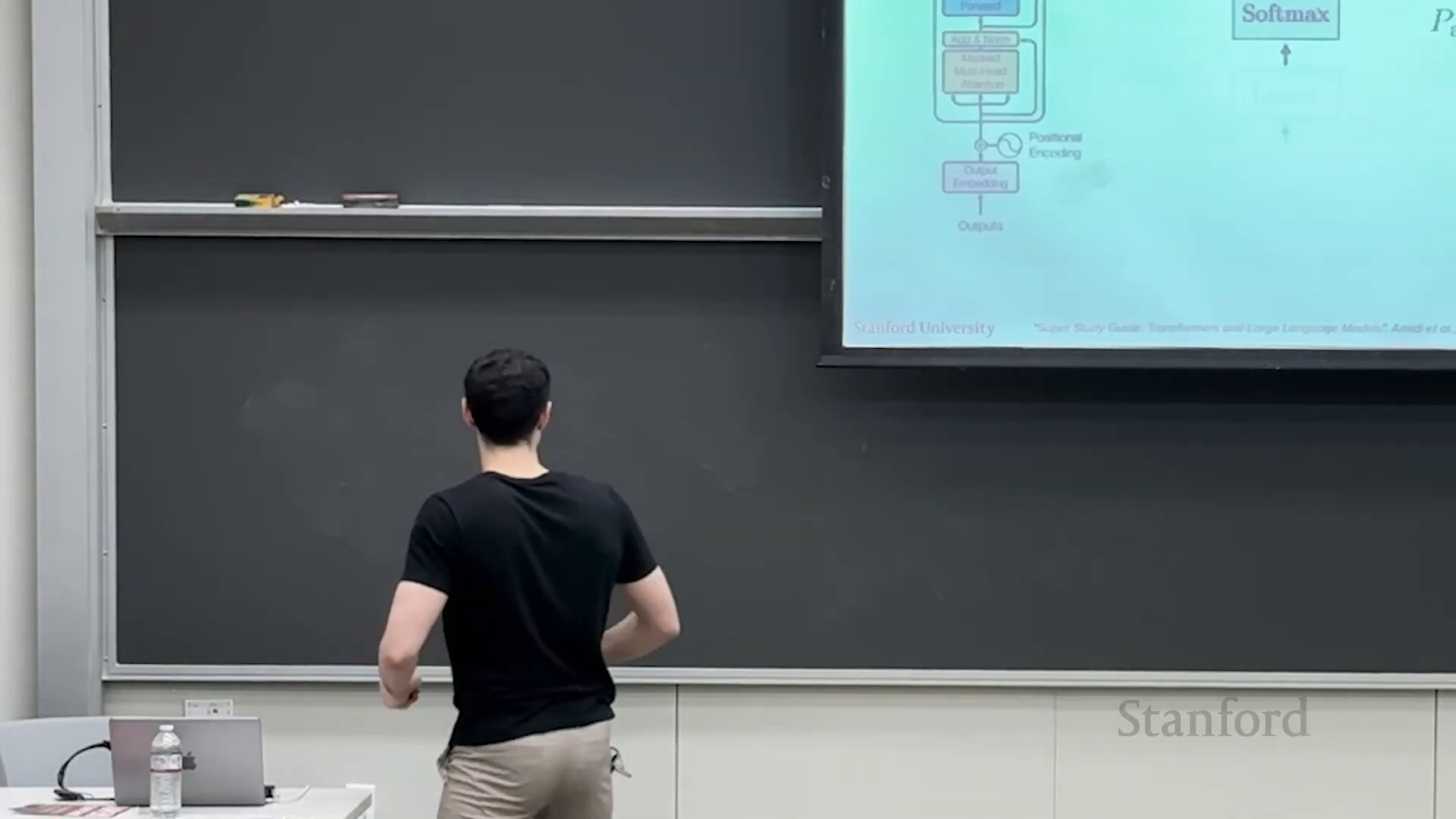
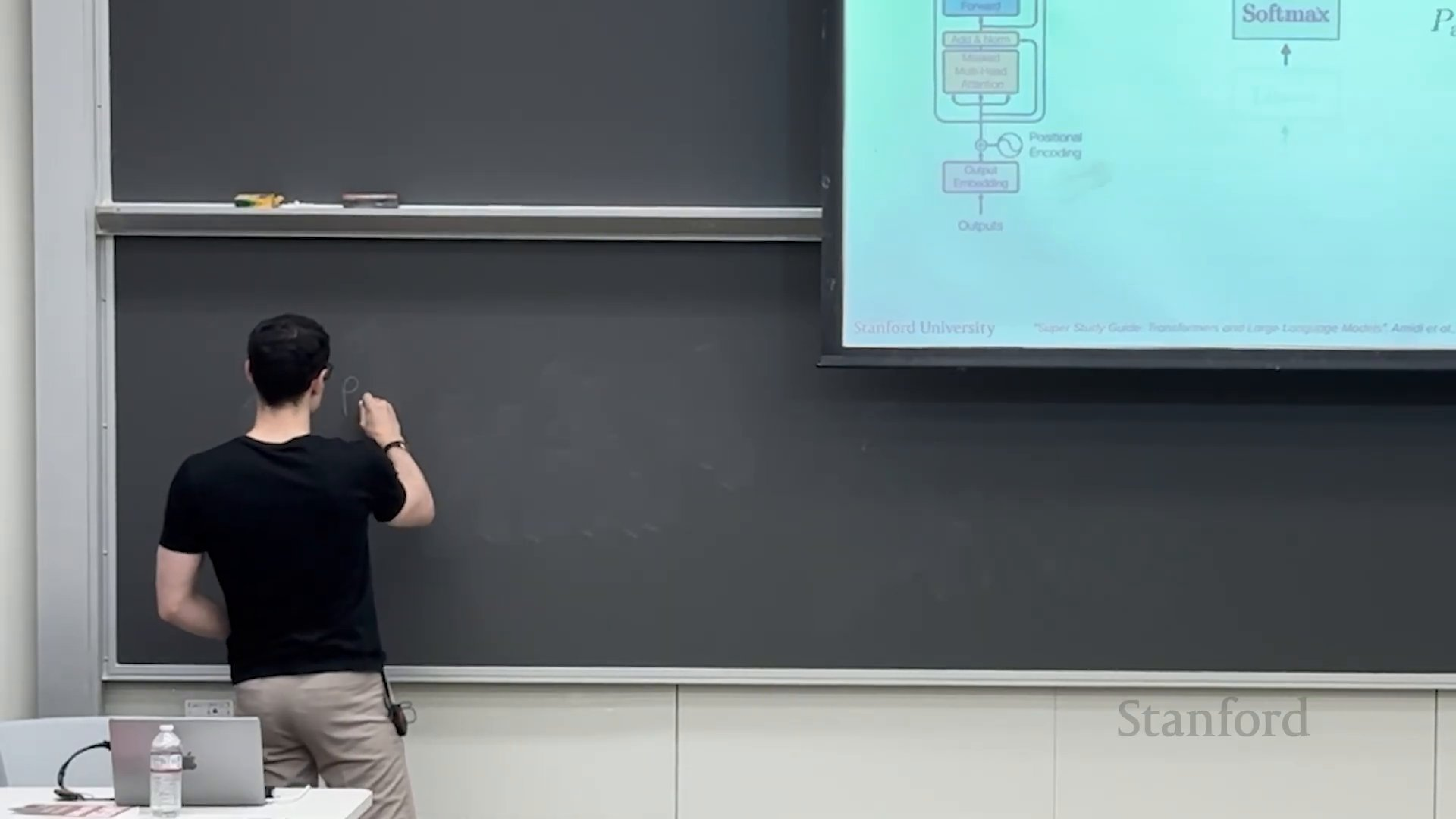

Forward
Add & Norm
Masked
Multi-Head
Attention
Positional
Encoding
Output
Embedding
Outputs
Softmax
Stanford University
"Super Study Guide: Transformers and Large Language Models", Amidi et al.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Add & Norm
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Multi-Head
Attention
Positional
Encoding
Output
Embedding
Outputs
Softmax
Stanford University
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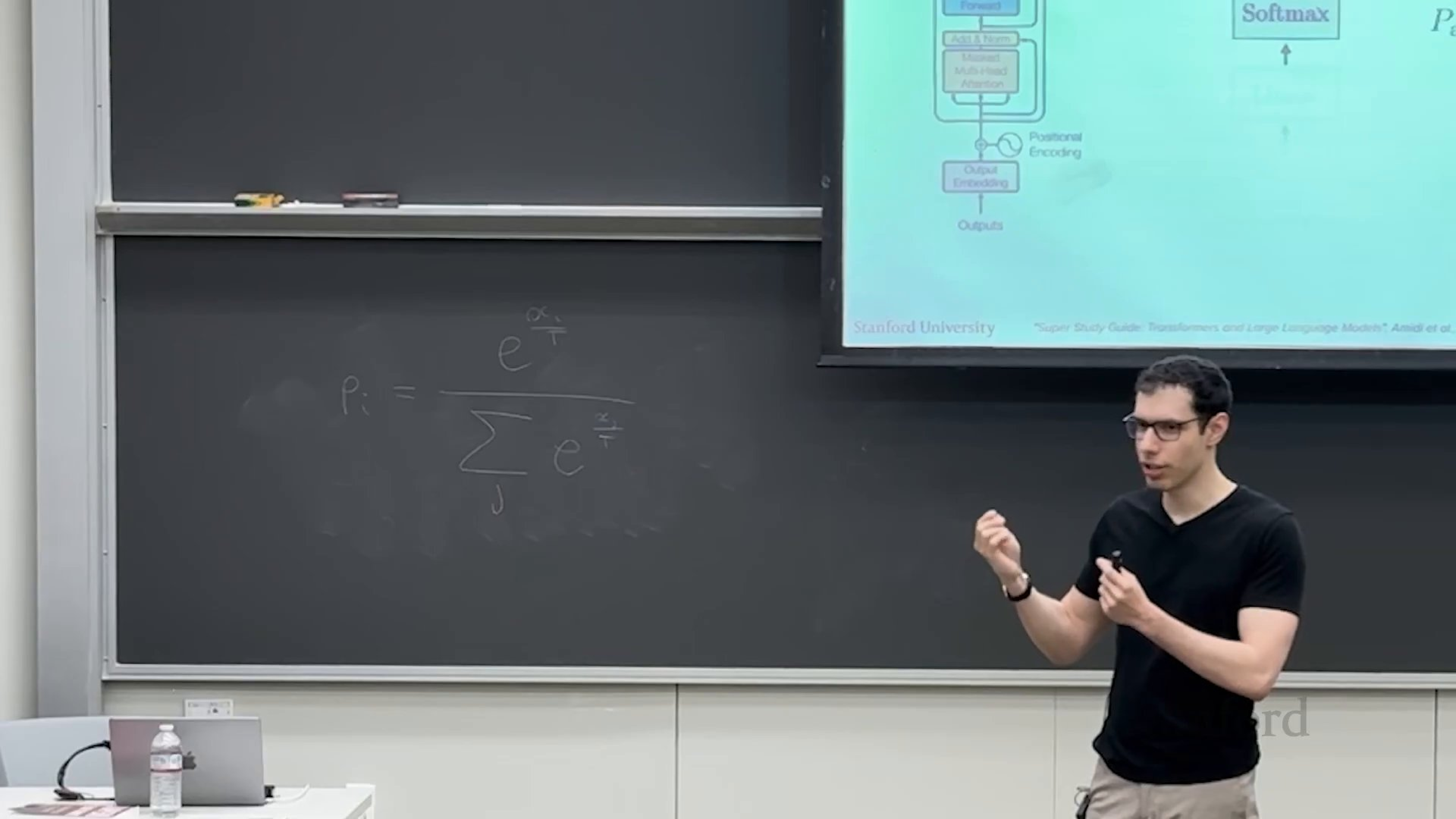
Stanford


Forward
Add & Norm
Masked Multi-Head Attention
Positional Encoding
Output Embedding
Outputs
Softmax
Stanford University
"Super Study Guide: Transformers and Large Language Models", Amidi et al.
$p_i = \frac{e^{\frac{x_i}{T}}}{\sum_j e^{\frac{x}{T}}}$
Stanford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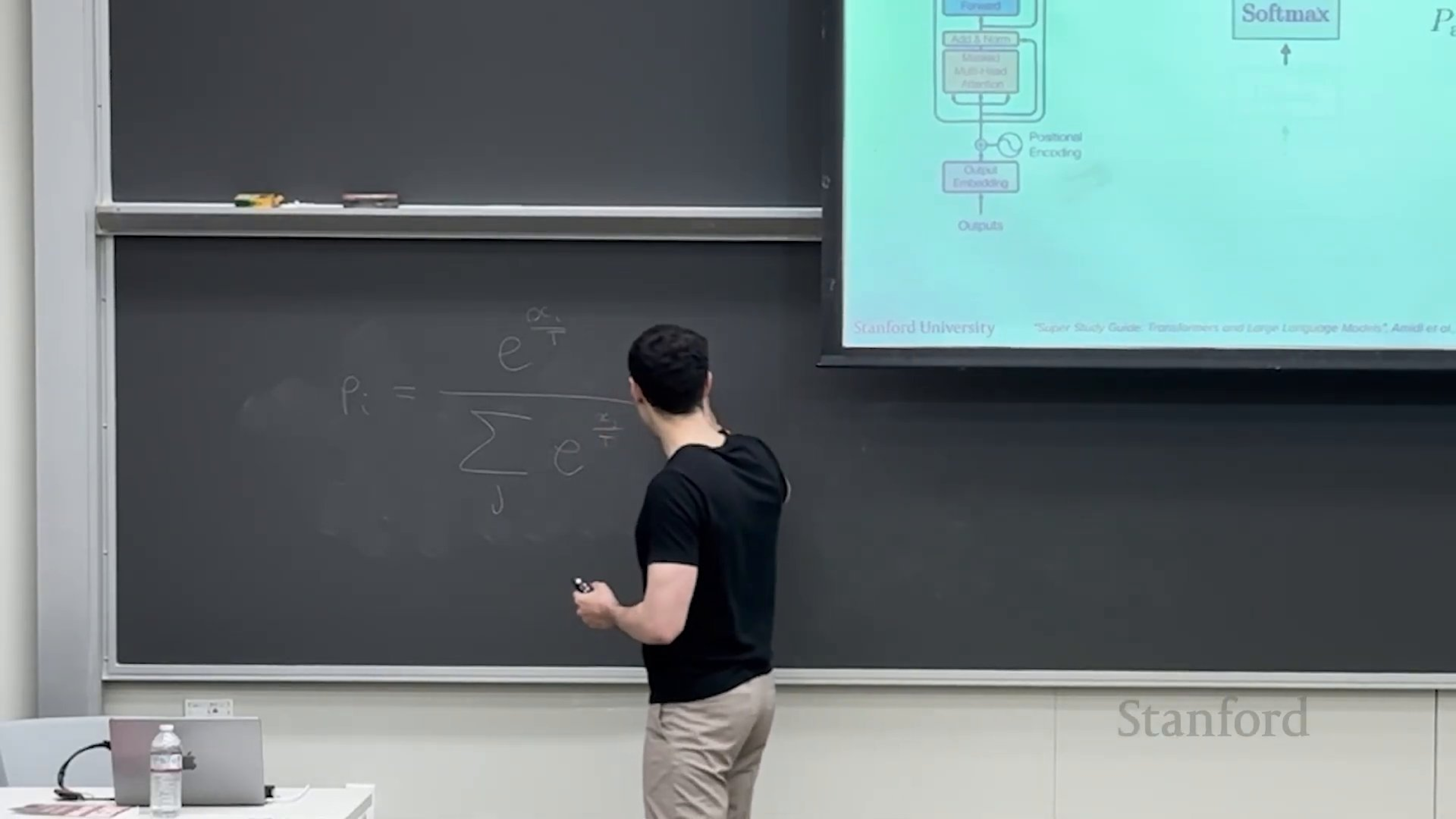
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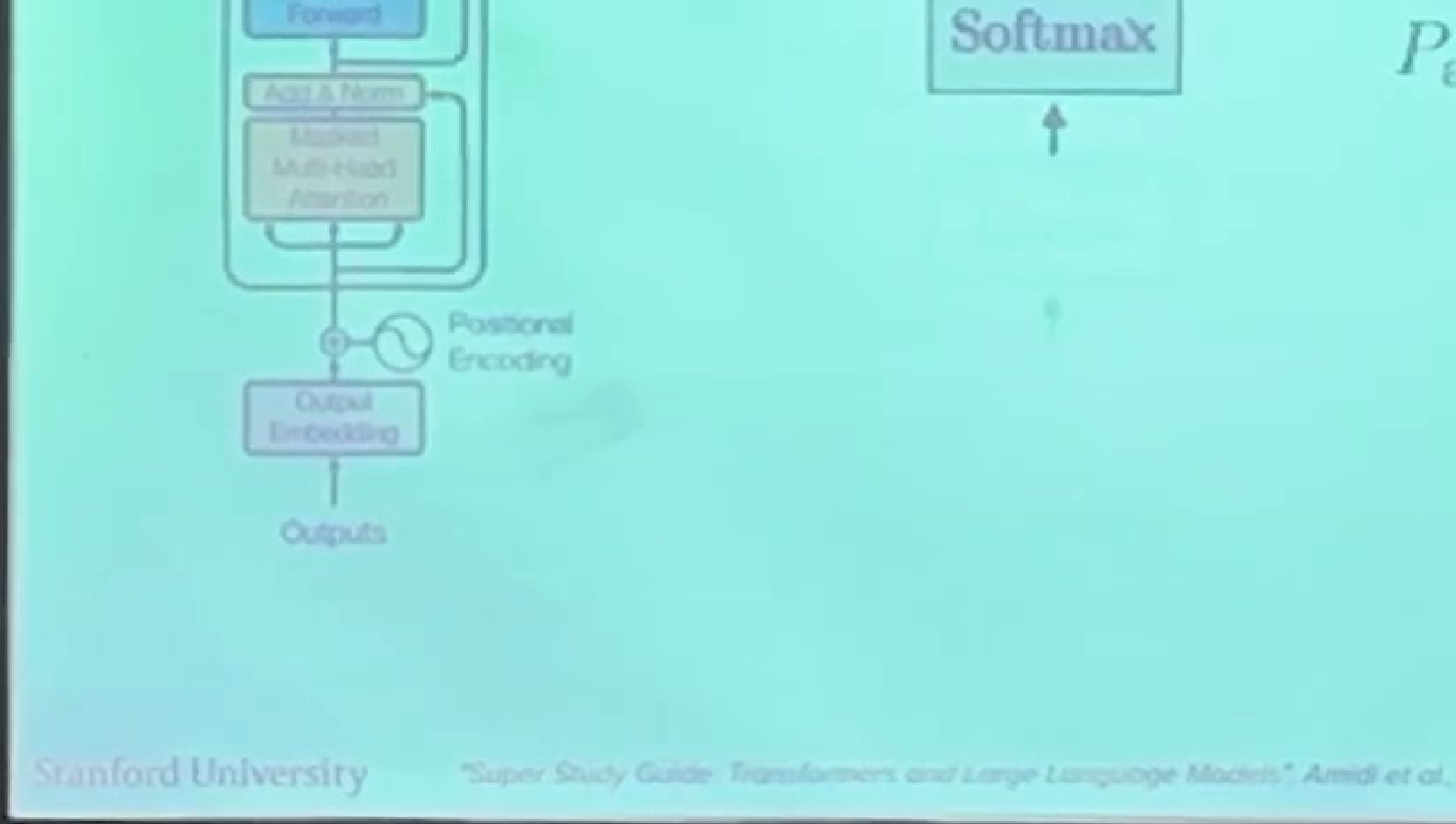

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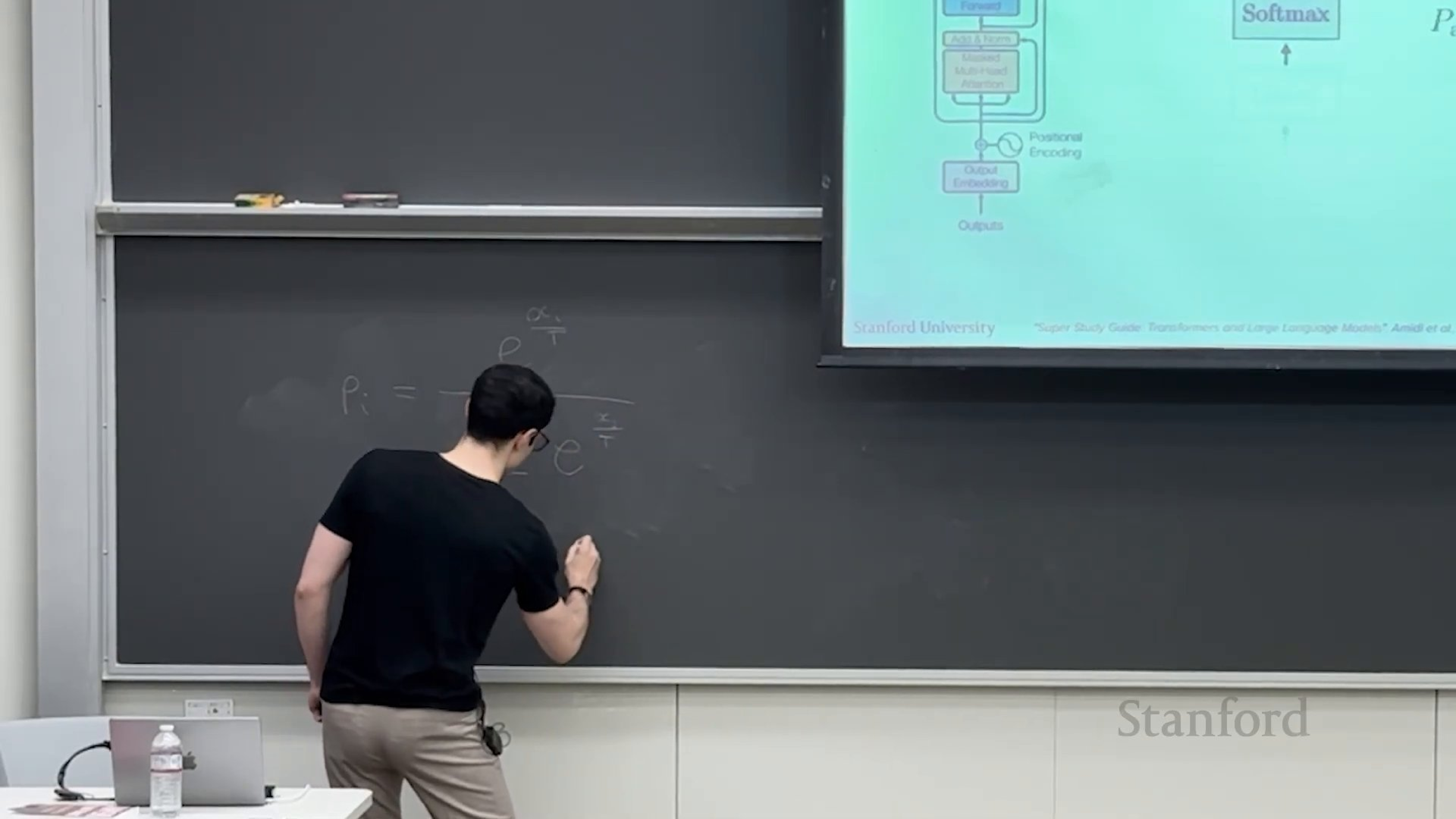
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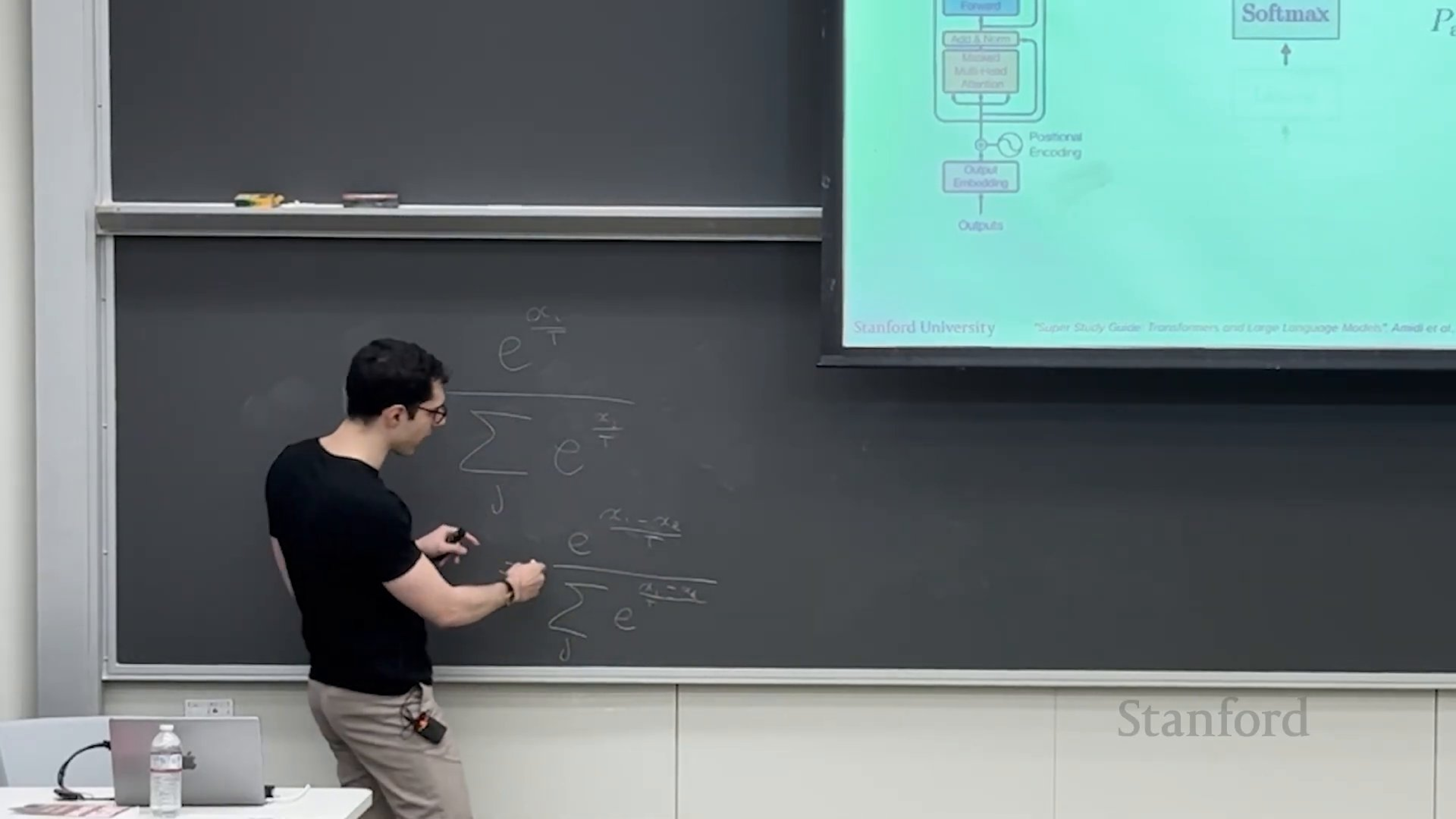

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$$\frac{e^{\frac{x_i - x_k}{T}}}{\sum_j e^{\frac{x_j - x_k}{T}}}$$
Stanford


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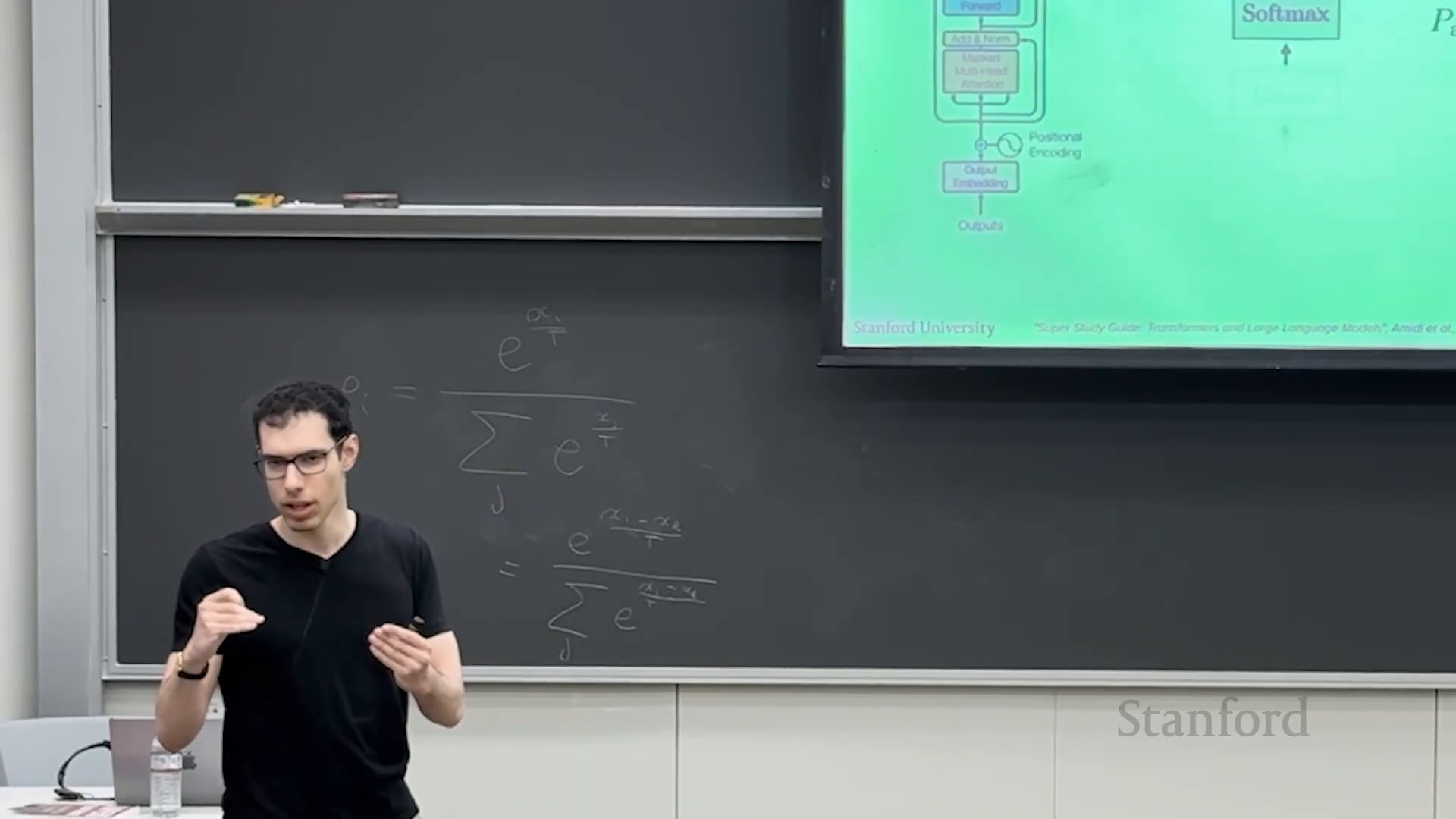
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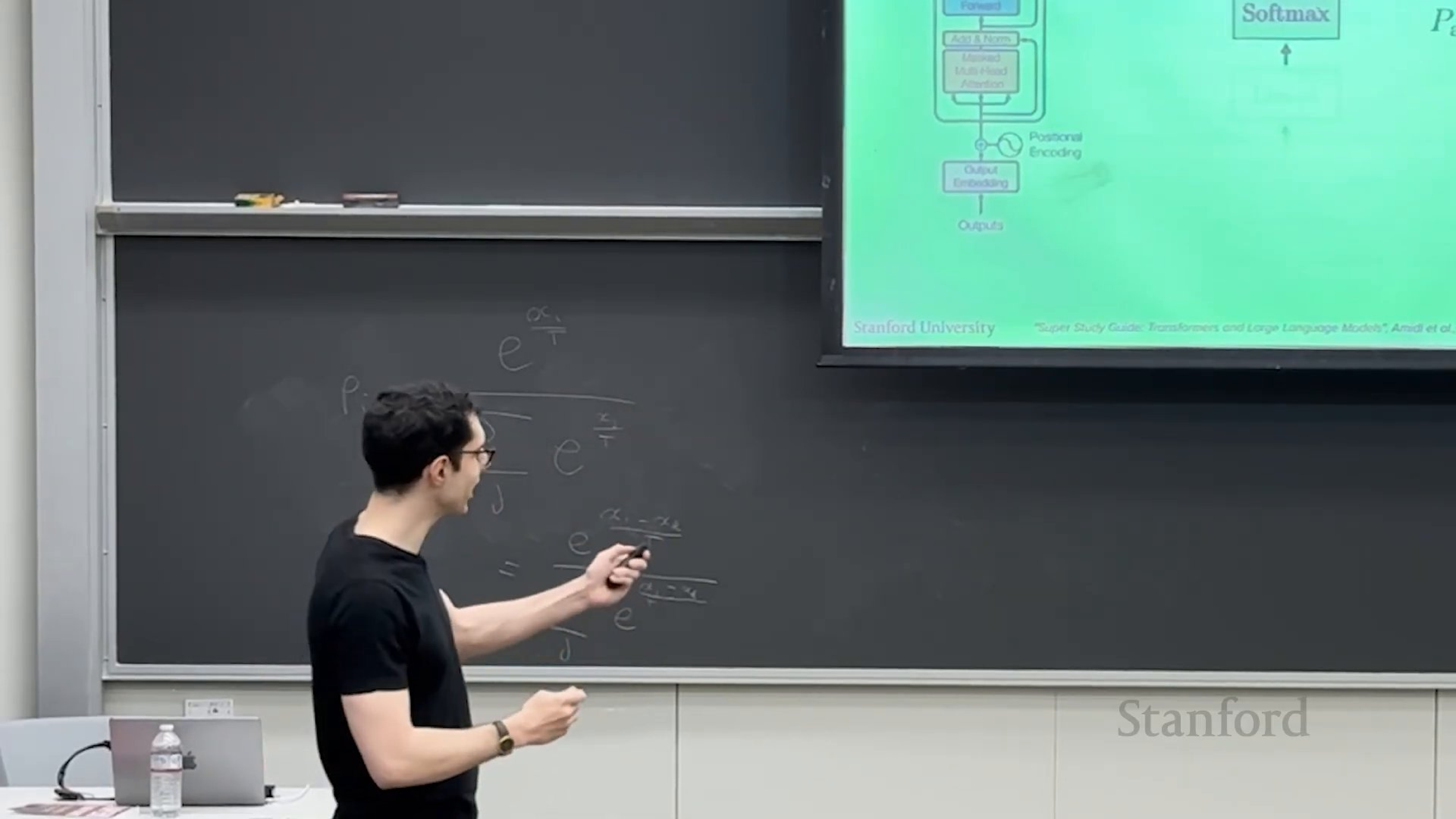
Stanford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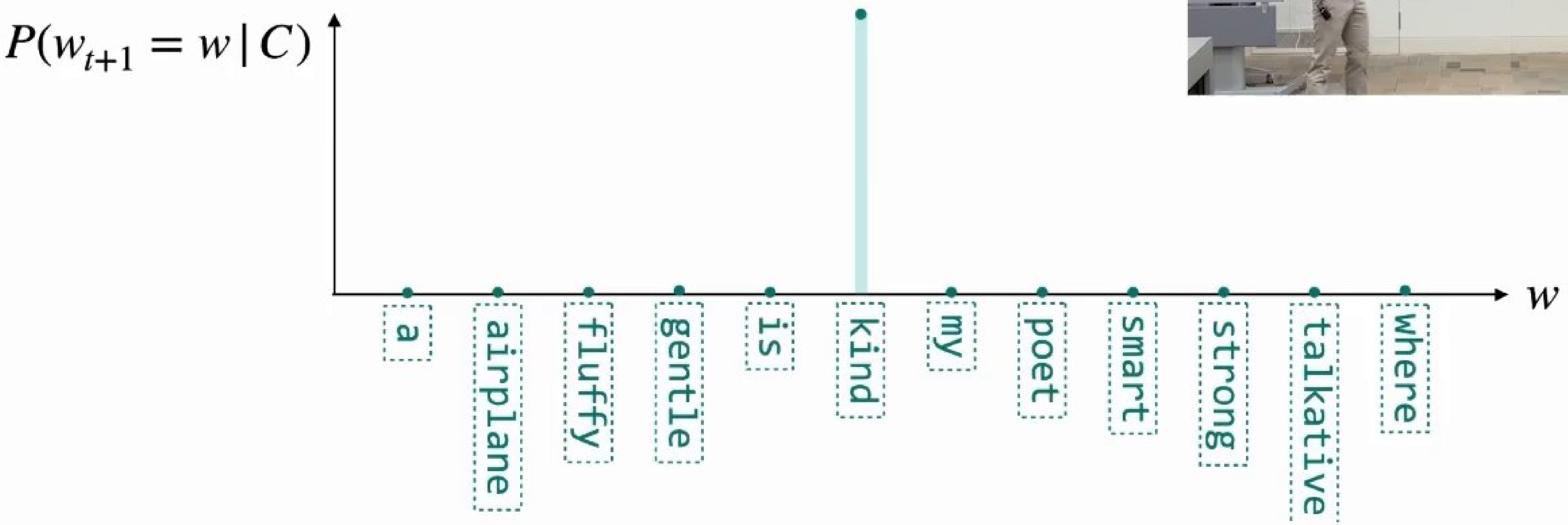
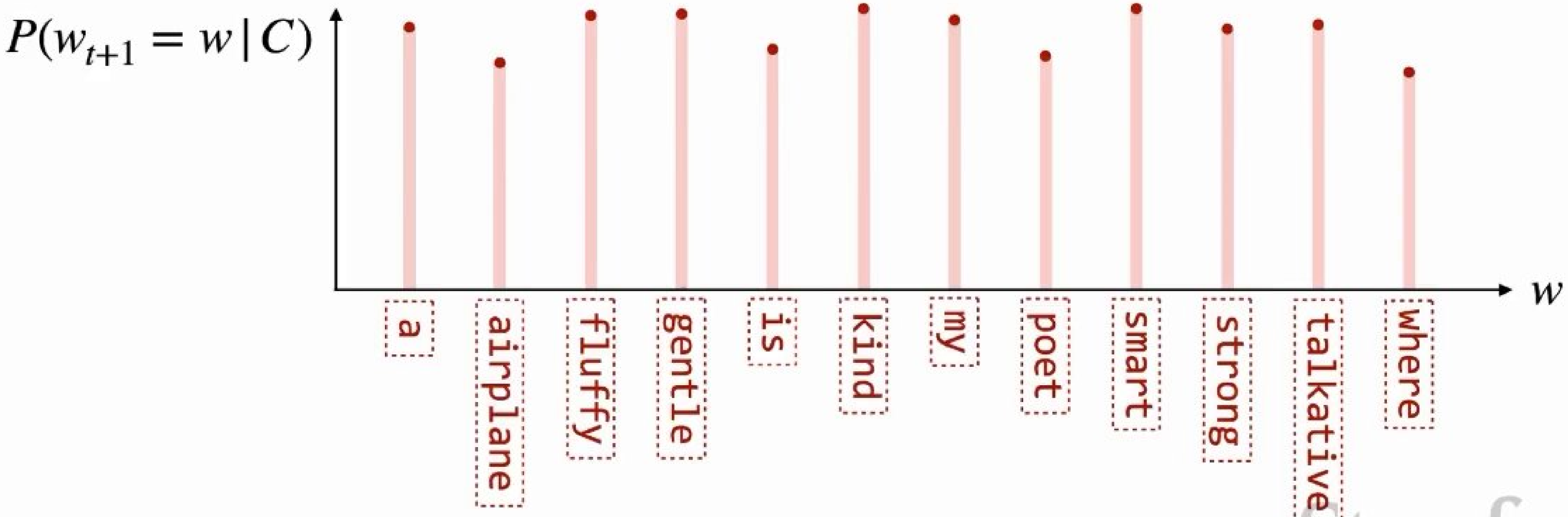
"Super Study Guide: Transformers and Large Language Models", Amidi et al.
Stanford

Impact of temperature on probabilities

Small T



High T



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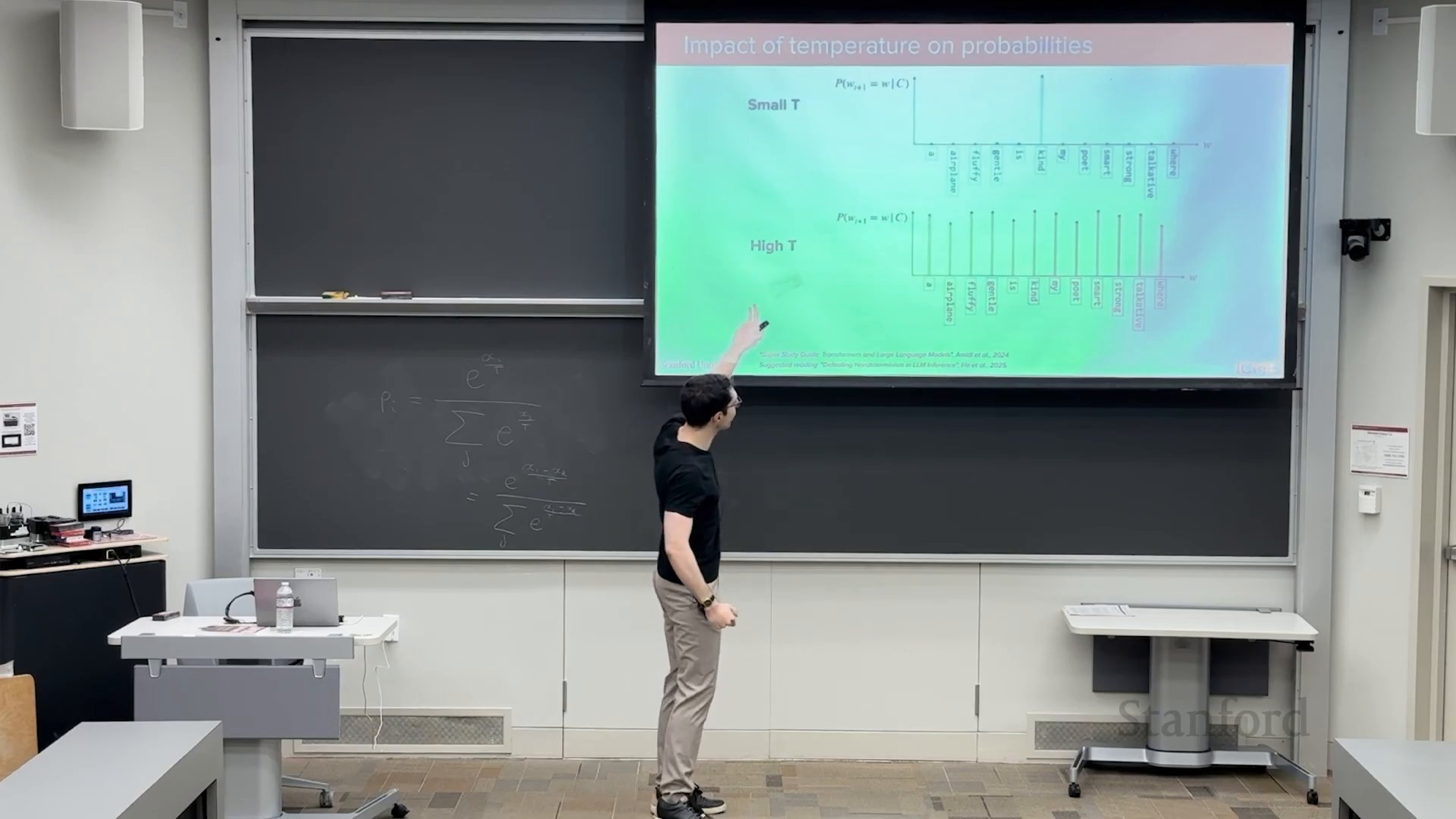

Impact of temperature on probabilities
Small T
$P(w_{i+1} = w \mid C)$
w
a
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talkative
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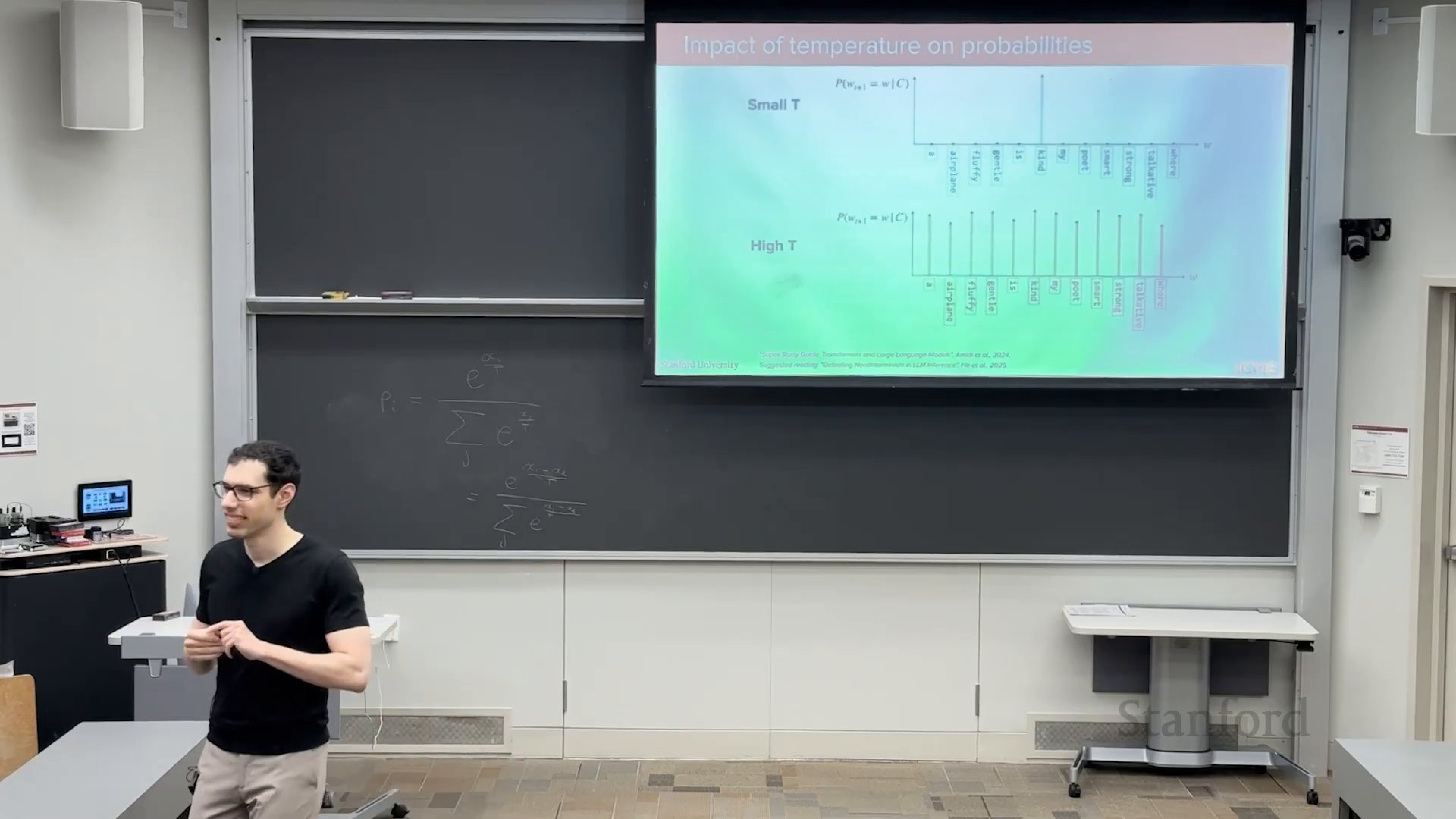
Stanford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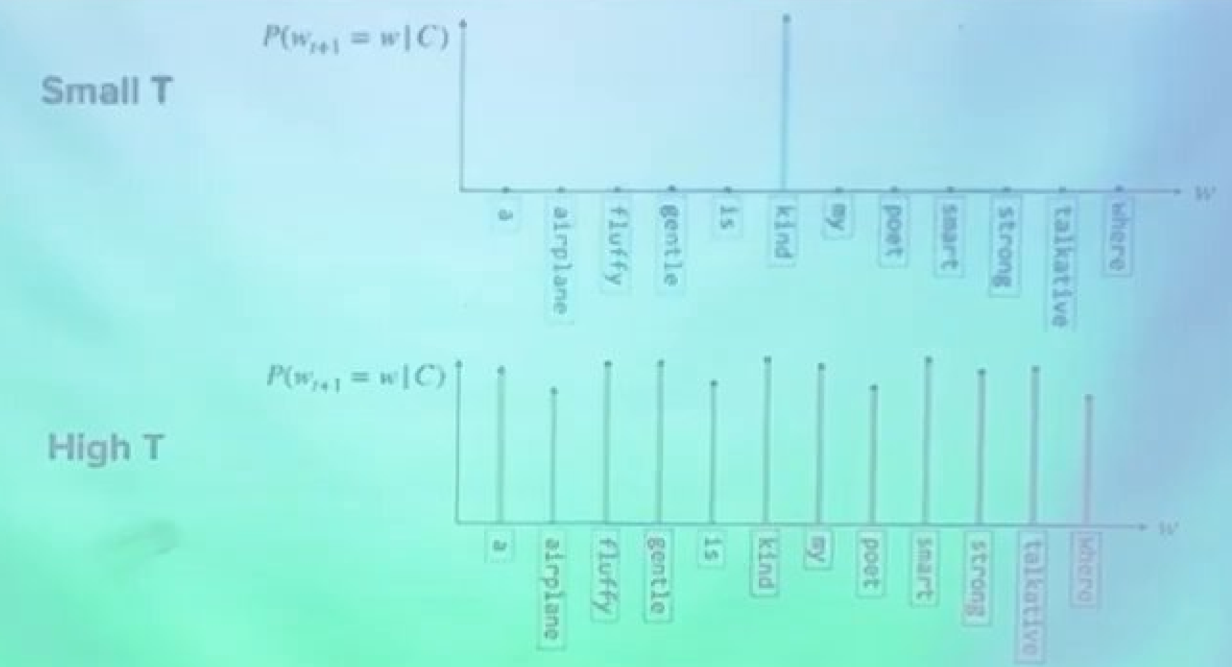
Impact of temperature on probabilities



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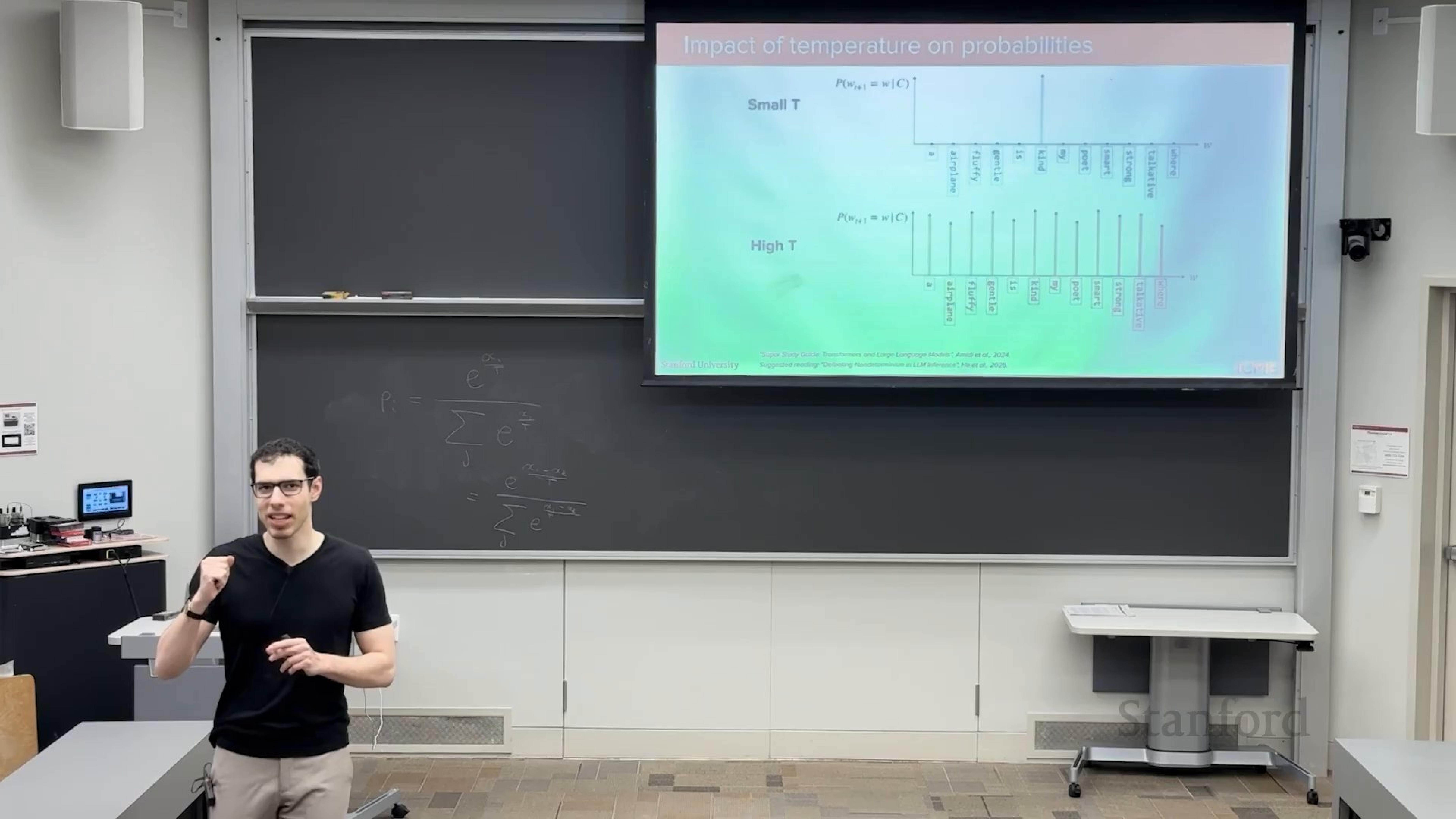
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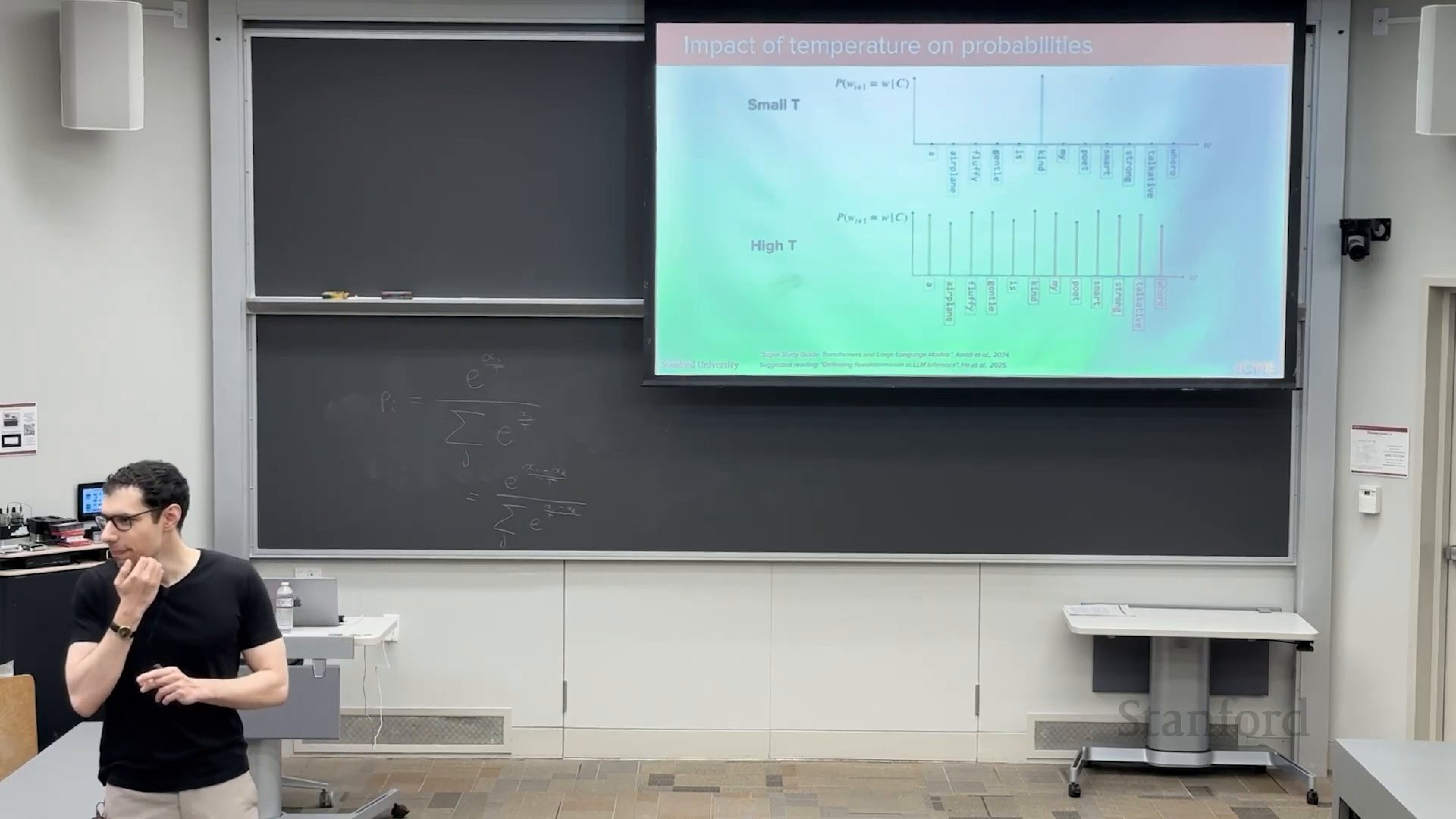
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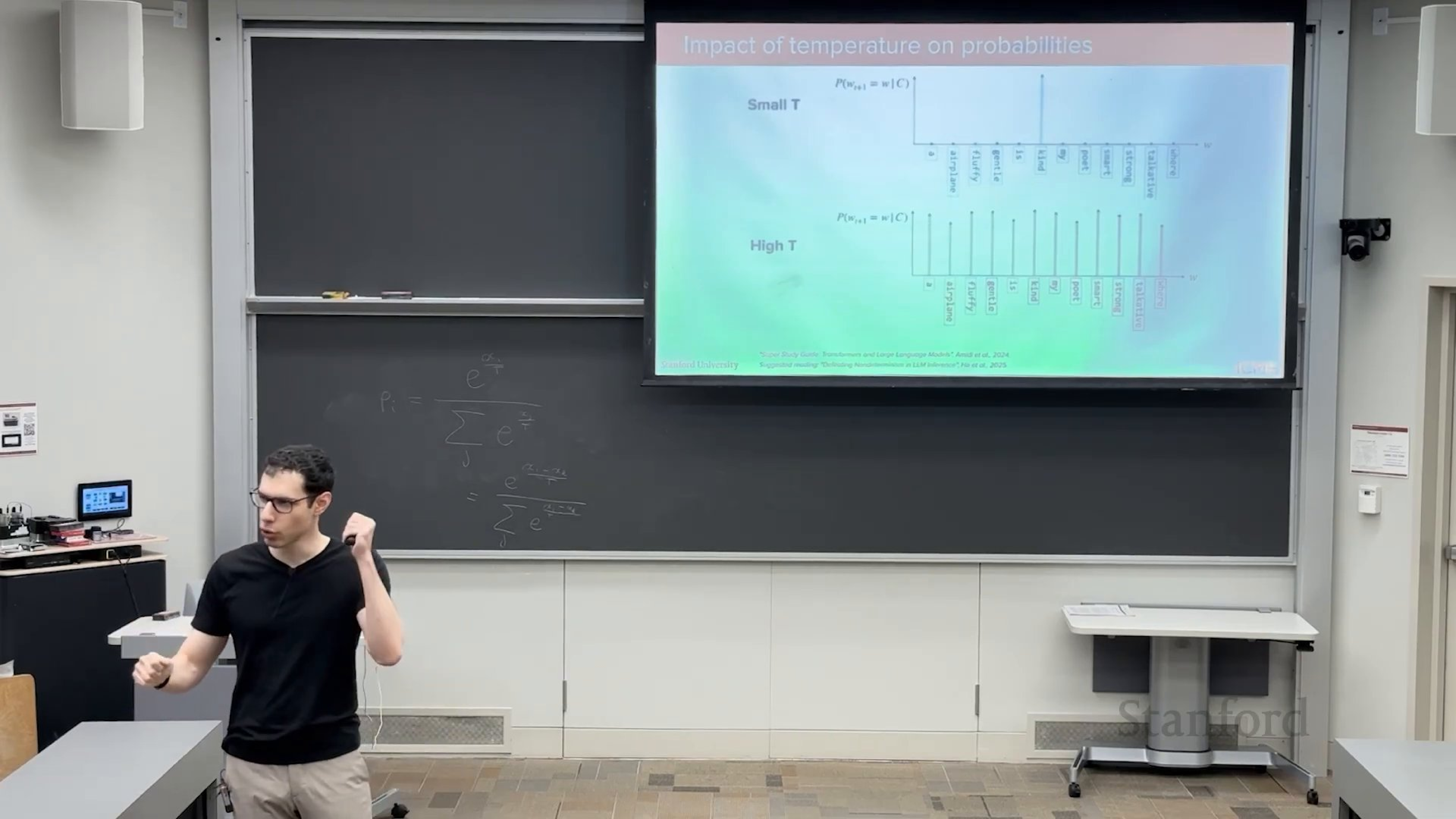

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Stanford University
ICME
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Stanford

Constraining the output via guided decod

Motivation. Generate output in a specific format

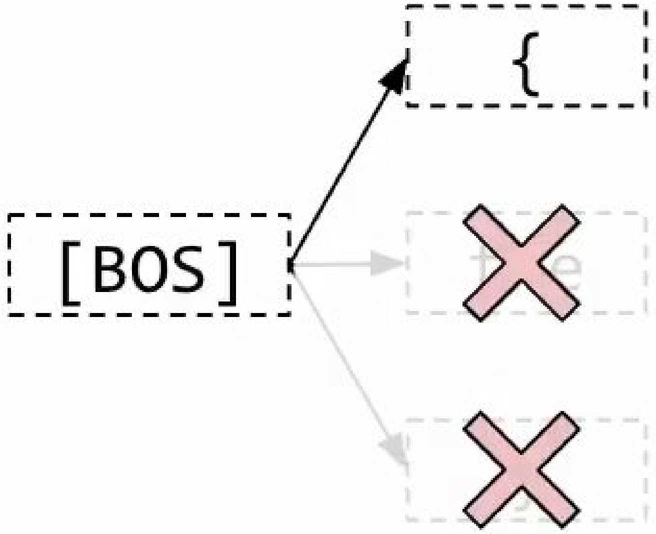
Input prompt
Generate a description of my 33-year old teddy bear who likes reading. *Do this in JSON format.*

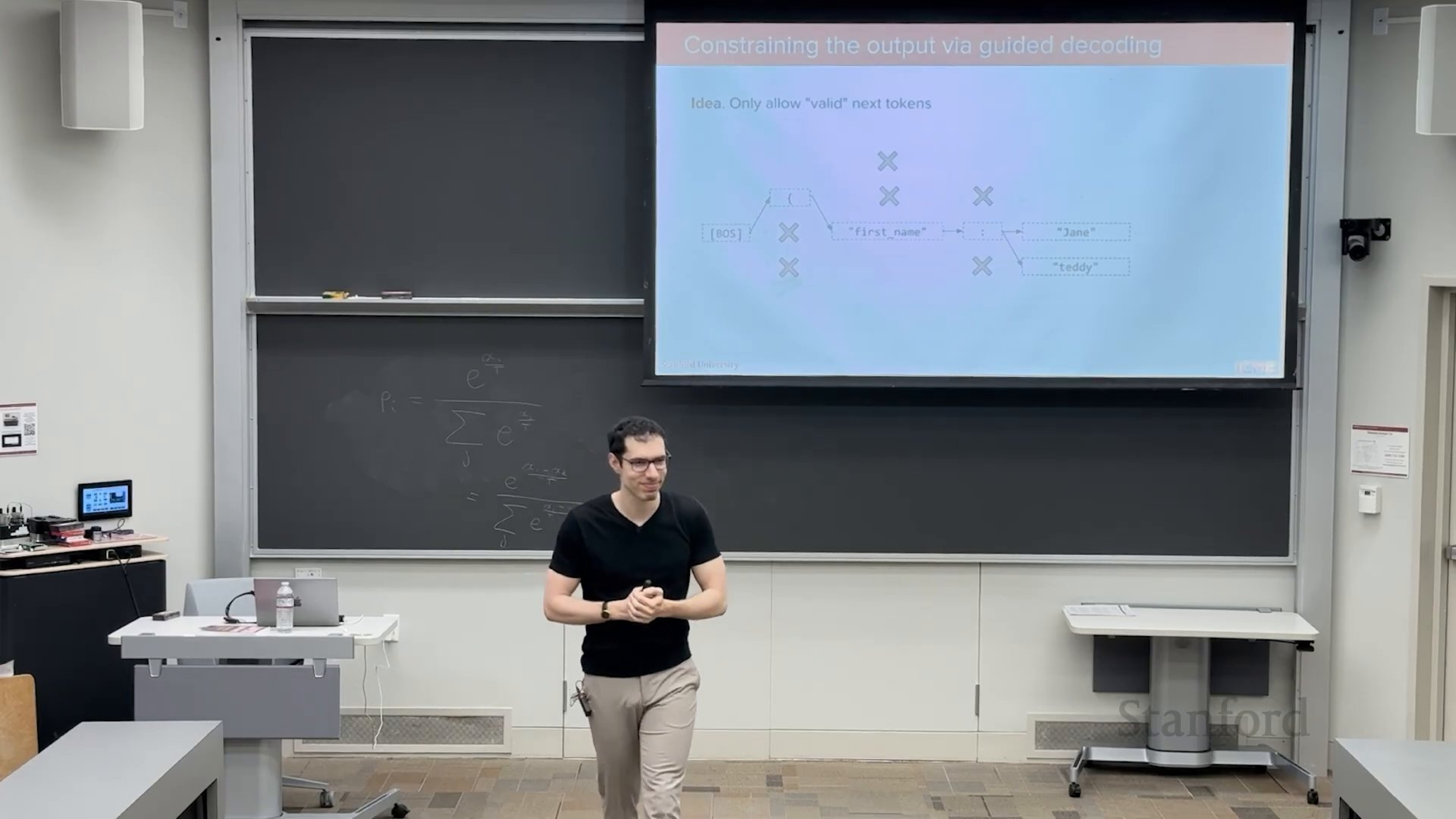
Desired output (JSON)

```json
{
    "first_name": "teddy",
    "last_name": "bear",
    "age": 33,
    "hobby": "reading"
}
```

Constraining the output via guided decod

Idea. Only allow "valid" next tokens




Constraining the output via guided decoding
Idea. Only allow "valid" next tokens
[BOS]
{
"first_name"
:
"Jane"
"teddy"
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Transformers &
Large Language
Models
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LLM overview
MoE-based LLMs
Response generation
Prompting strategies
Inference optimizations
Stanford

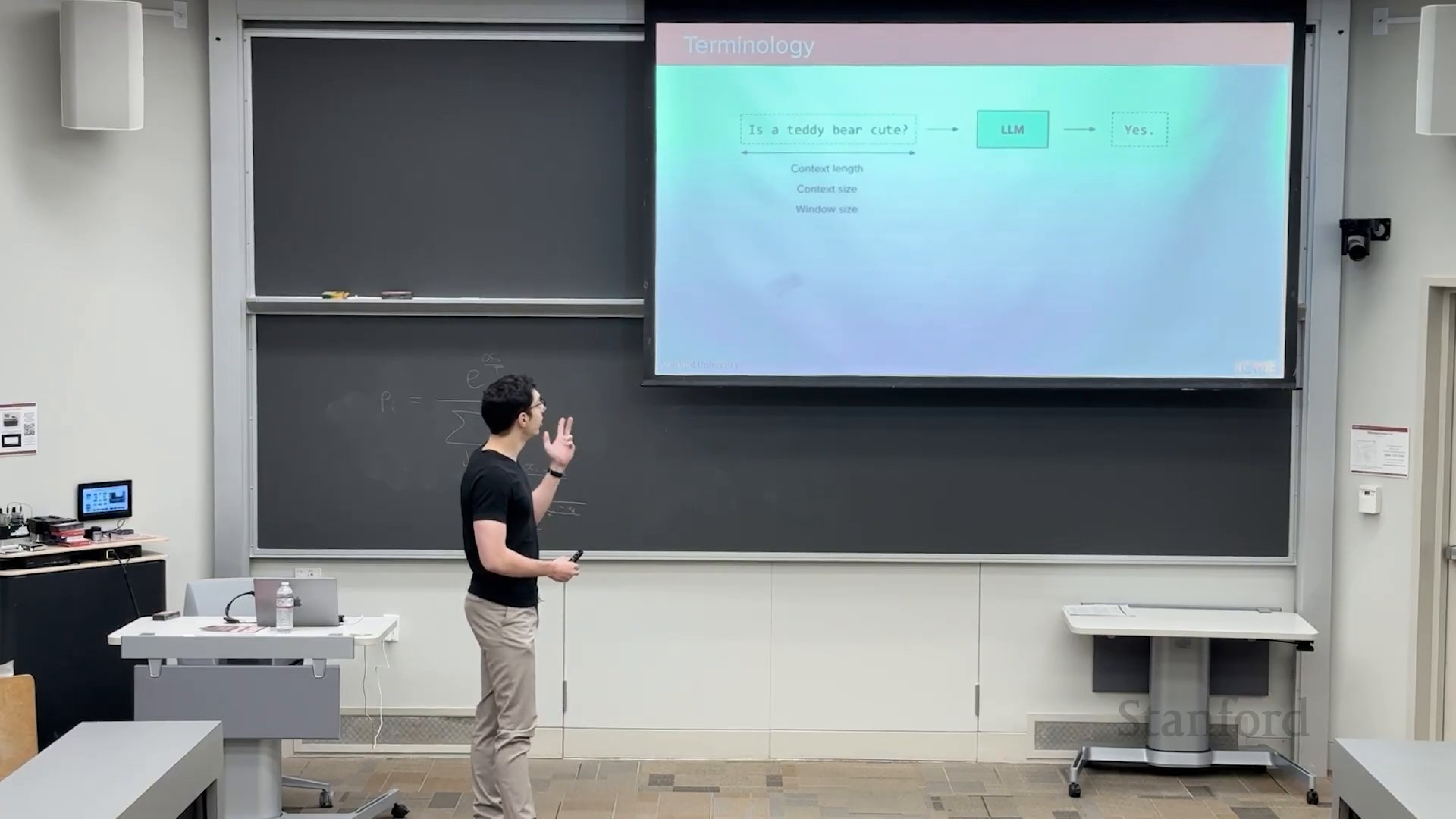
Terminology

`Is a teddy bear cute?` → **LLM** → `Yes.`

Context length

Context size

Window size


Terminology
Is a teddy bear cute?
LLM
Yes.
Context length
Context size
Window size
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Terminology

`Is a teddy bear cute?` → **LLM** → `Yes.`

Context length

Context size

Window size

Discussion. Orders of magnitude by:

- Input type
- Models

Stanford


Terminology
Discussion. Orders of magnitude by:
Input type
Models
Beware of "context rot"!
Stanford University
"Context Rot: How Increasing Input Tokens Impacts LLM Performance", Hong et al., 2025
Stanford

Main structure

My teddy bear had a long day and needs a bedtime story. — **Context**

Generate a bedtime story that takes place in a specific location. — **Instructions**

Location: Country of teddy bears — **Input**

The story needs to be suitable for teddy bears that are tired. — **Constraints**

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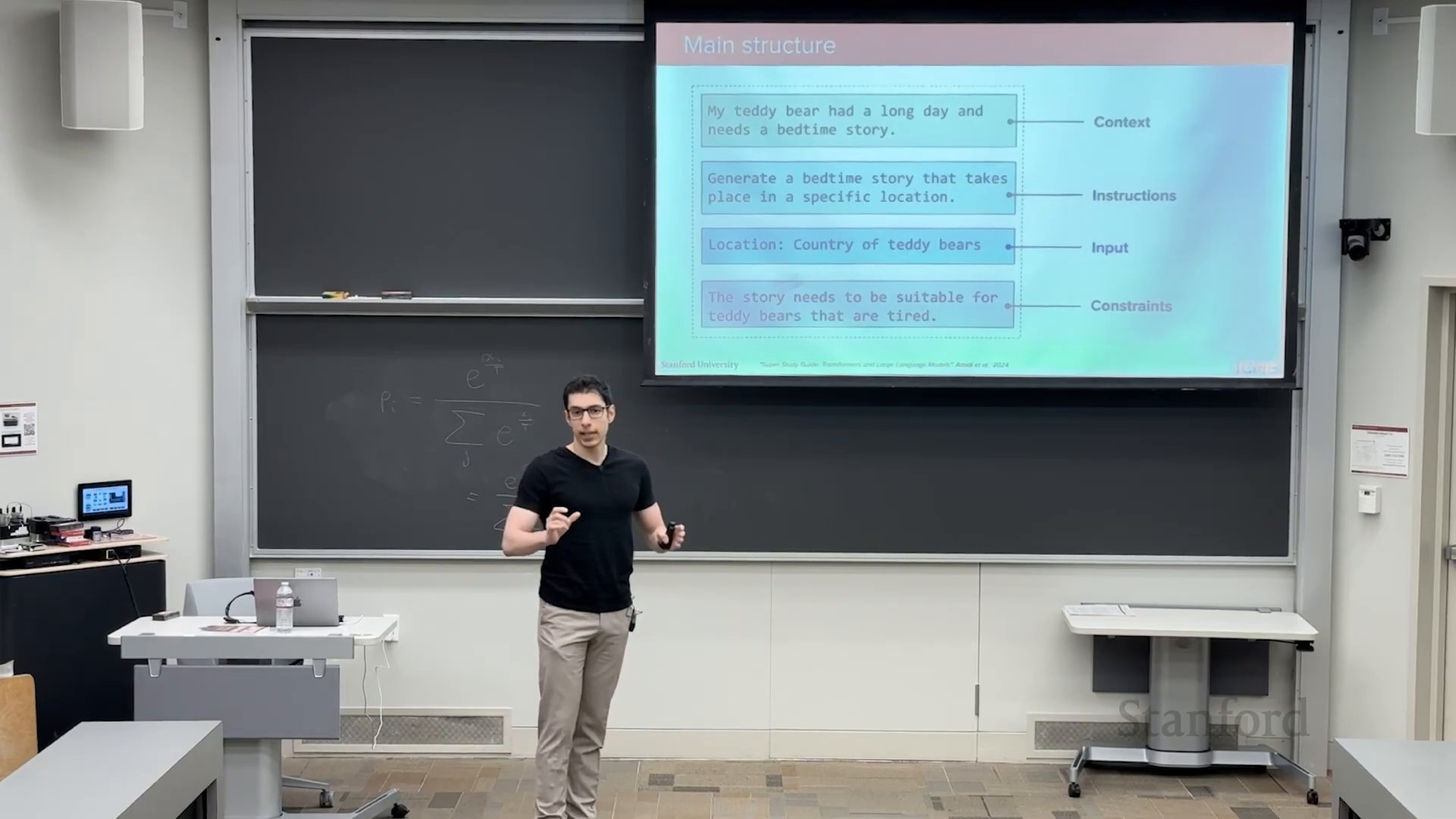
Main structure
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Generate a bedtime story that takes place in a specific location.
Instructions
Location: Country of teddy bears
Input
The story needs to be suitable for teddy bears that are tired.
Constraints
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In-context learning

ICL = **I**n-**C**ontext **L**earning

Stanford


In-context learning
ICL = In-Context Learning
Stanford University
"Language Models are Few-Shot Learners" Brown et al., 2020
Stanford

In-context learning

ICL = In-Context Learning

Zero-shot learning	Few-shot learning
• Question is asked without examples • Performance heavily depends on performance of initial model	• Prompt contains examples of input / output • Typically has a better performance

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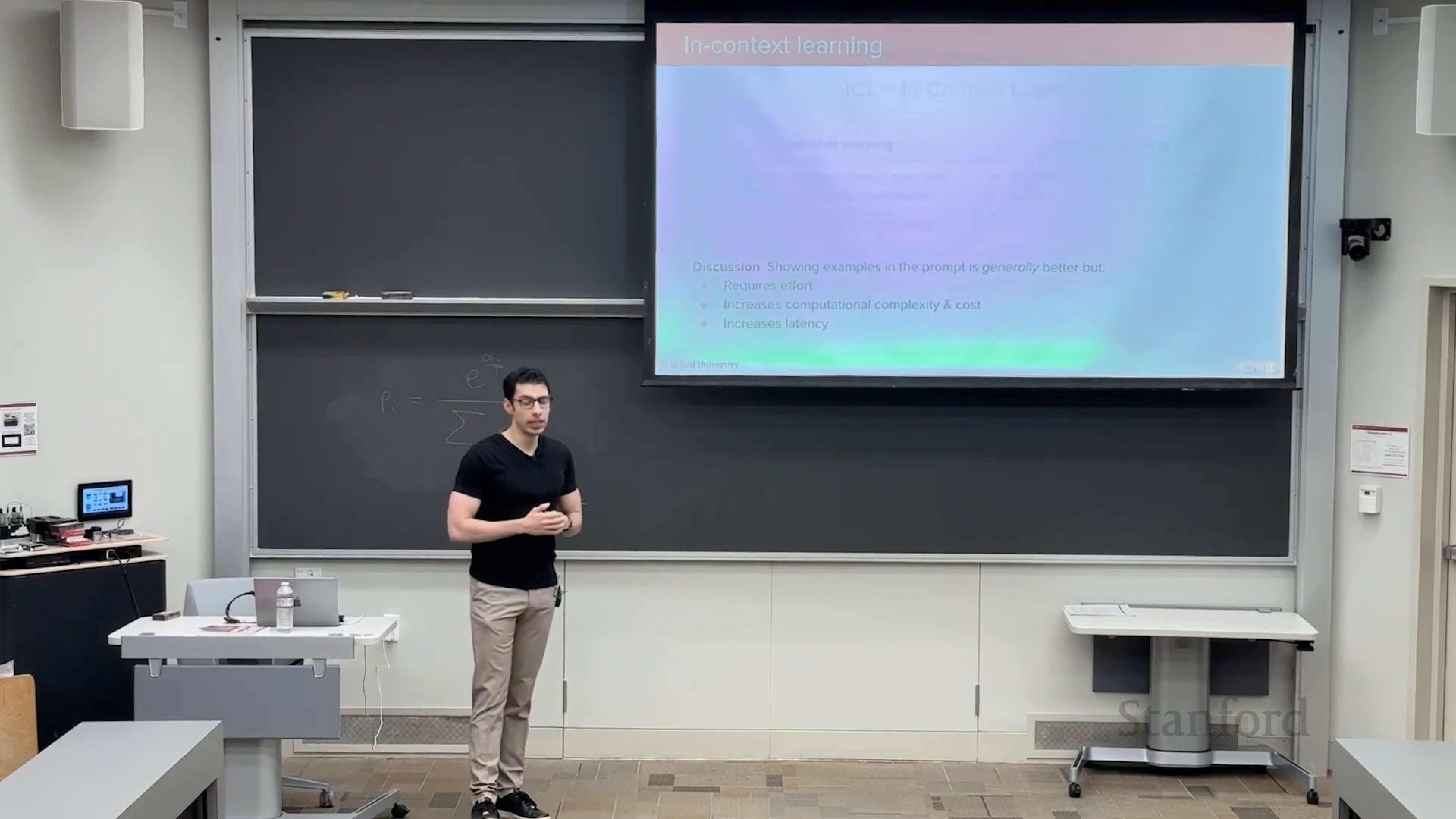
In-context learning
Discussion. Showing examples in the prompt is *generally* better but:
Requires effort
Increases computational complexity & cost
Increases latency
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Stanford

Chain of thought

Idea. Explaining reasoning helps in improving performance.

```
Q: How old is this bear?
A: The bear was born in
2020. It is therefore 4.


Q: How old will the bear
be next year?
```

→ LLM →

```
A: It will be one
year older than
its age this year,
which was 4.
Hence, it will be
5.
```

Discussion.

- Interpretability + explanation
- More tokens: higher cost and latency

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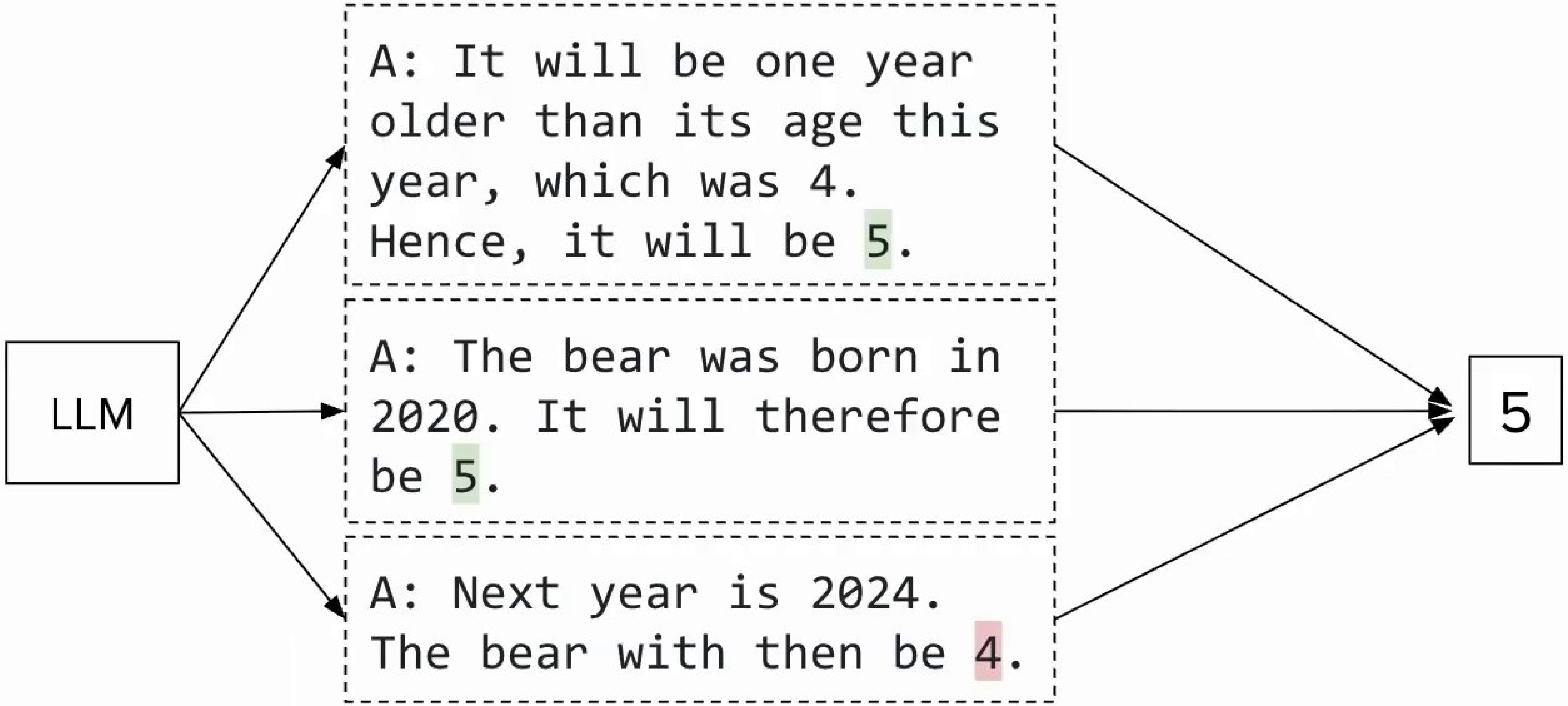
Self-consistency

Idea. Aggregating over reasoning paths improves performance.



Discussion. Trade-off between performance and added cost.

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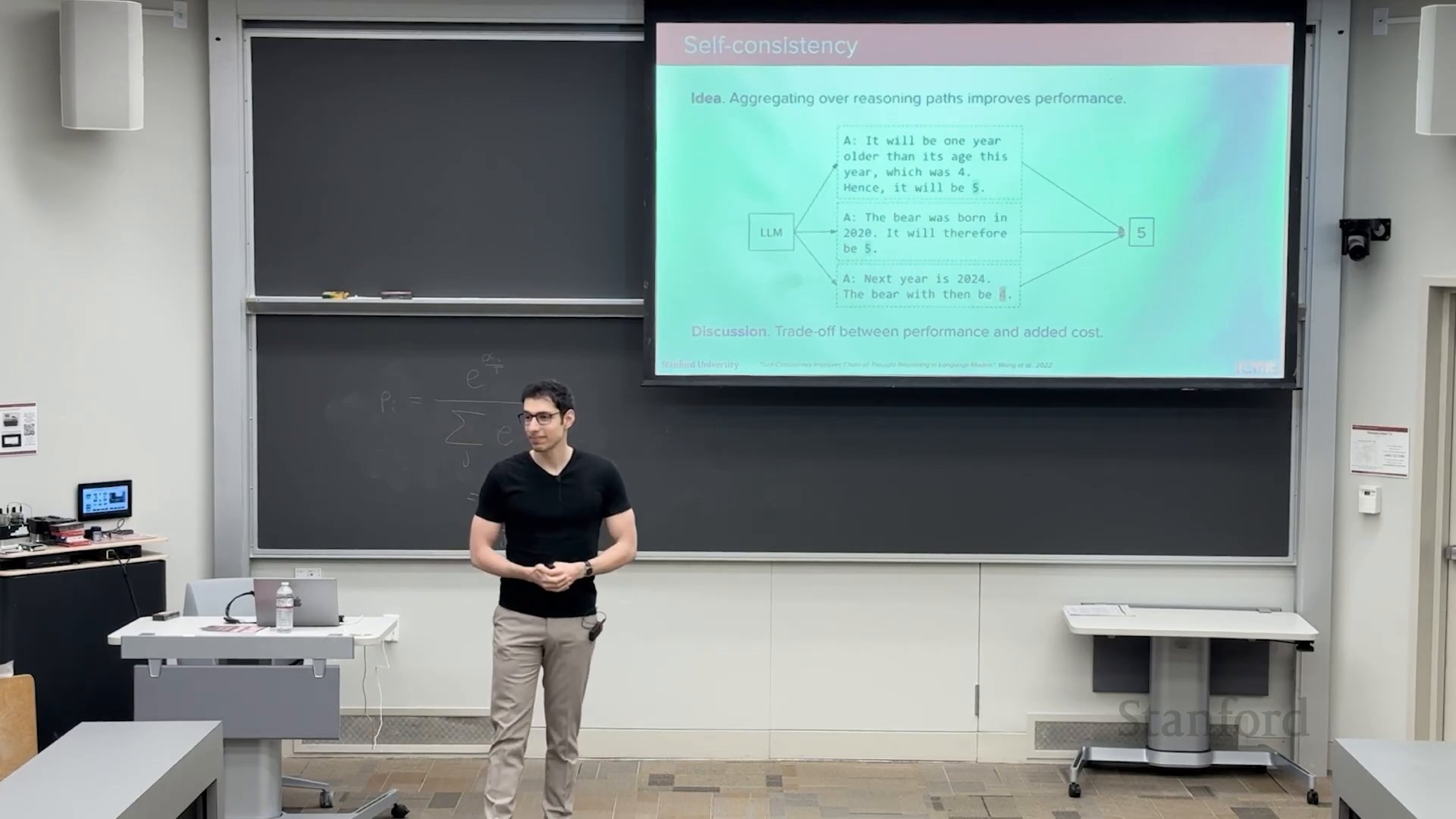

Self-consistency
Idea. Aggregating over reasoning paths improves performance.
LLM
A: It will be one year older than its age this year, which was 4. Hence, it will be 5.
A: The bear was born in 2020. It will therefore be 5.
A: Next year is 2024. The bear with then be 4.
5
Discussion. Trade-off between performance and added cost.
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Wang et al., 2022
ICME
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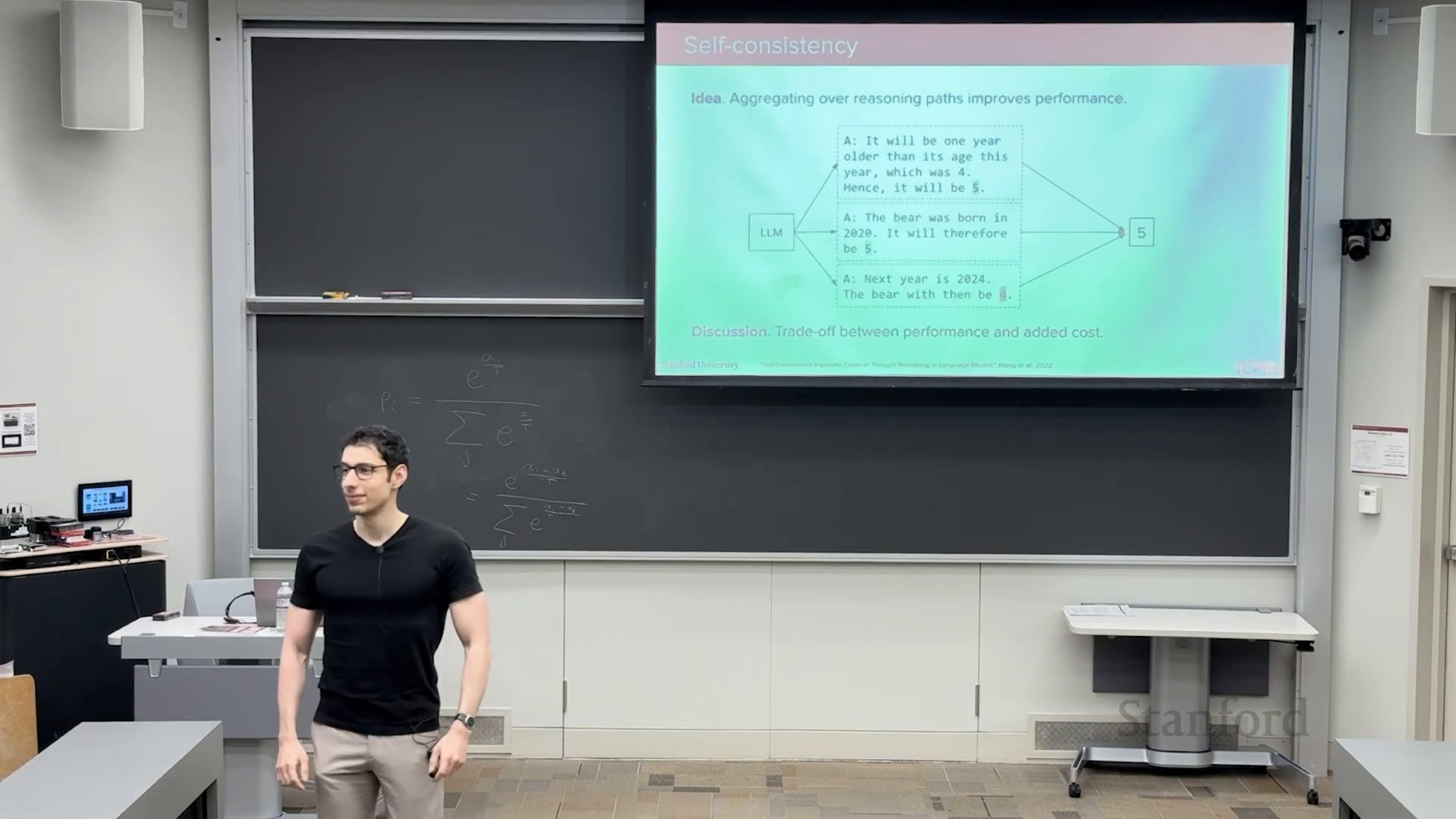
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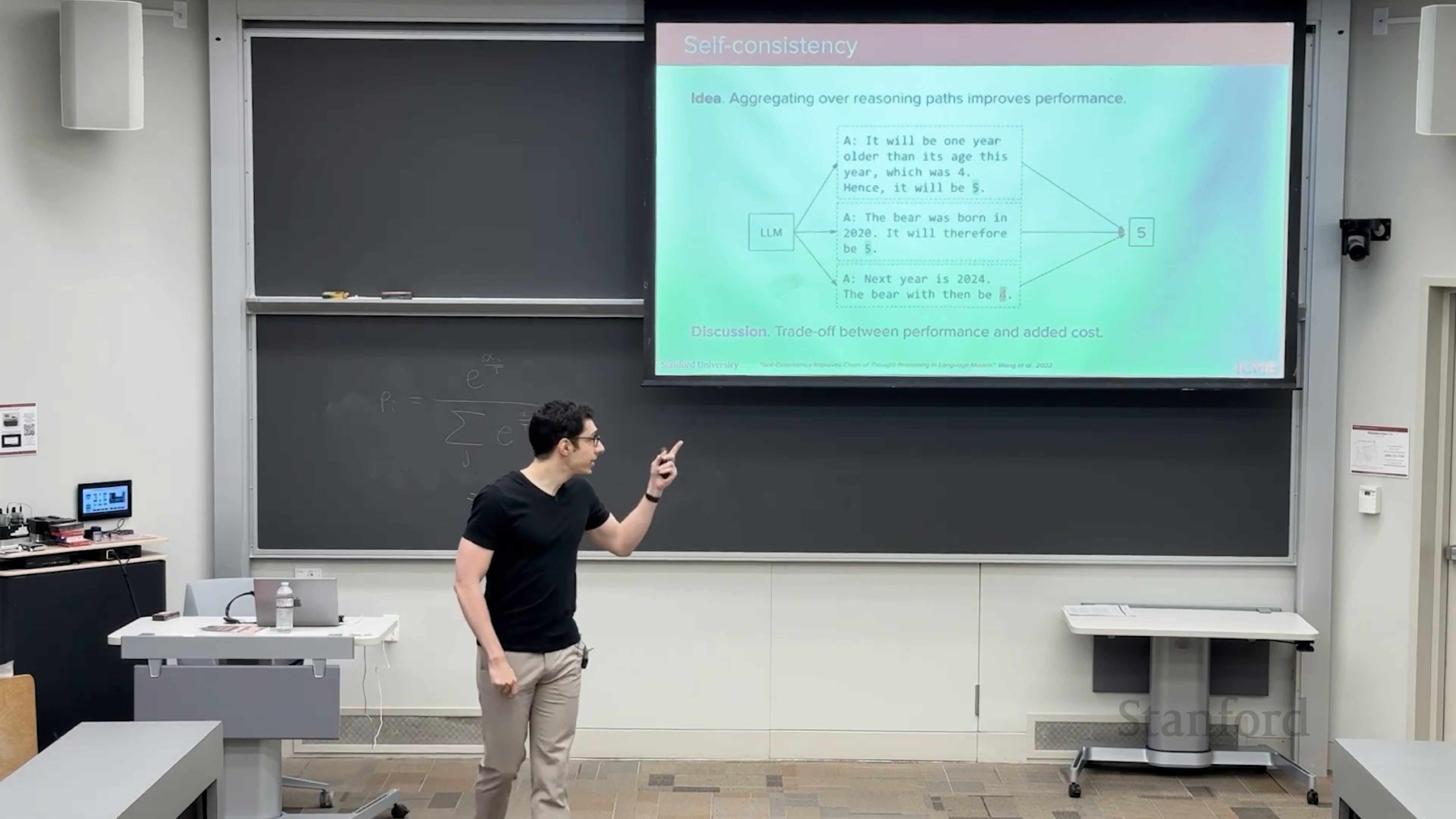
Discussion. Trade-off between performance and added cost.
Stanford University
"Self-Consistency Improves Chain of Thought Reasoning in Language Models" Wang et al. 2022
ICME
Stanford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ICME
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Transformers & Large Language Models

LLM overview

MoE-based LLMs

Response generation

Prompting strategies

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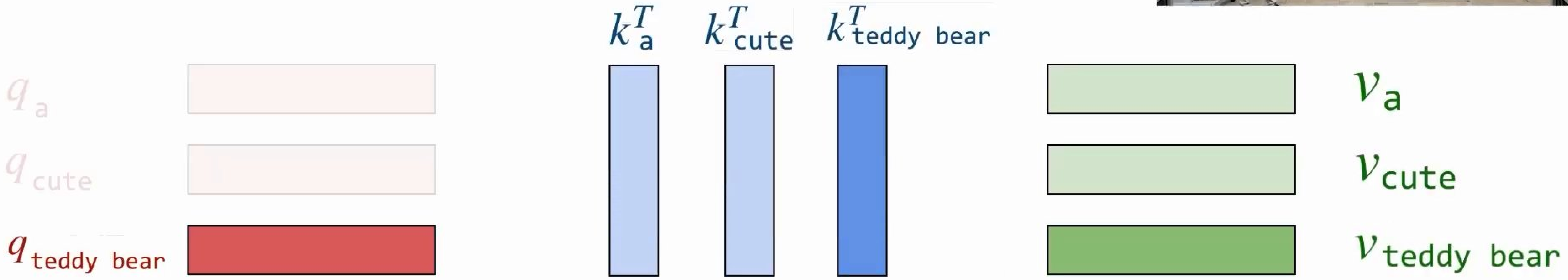
Challenges

Motivation. Computations are expensive, any way to reduce co

Categories. Many dimensions to optimize for.

Sharing attention heads




Sharing attention heads
k_a^T
k_{cute}^T
$k_{teddy\ bear}^T$
v_a
v_{cute}
$v_{teddy\ bear}$
$q_{teddy\ bear}$
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Sharing attention heads

Idea. Share key/value attention heads within groups of queries

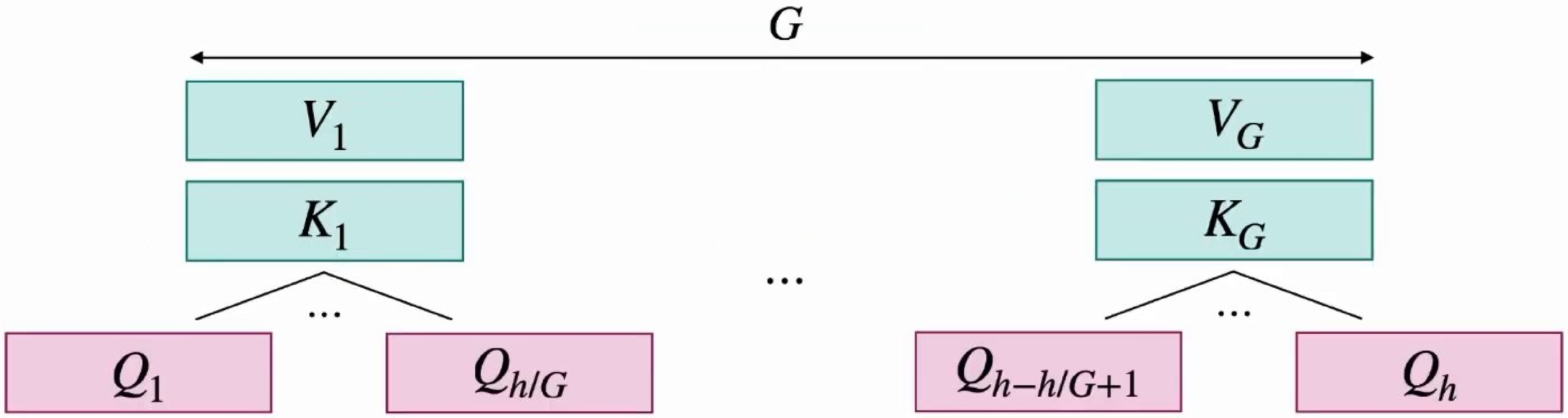


Figure from "Super Study Guide: Transformers & Large Language Models", Amidi et al., 2024.

Sharing attention heads

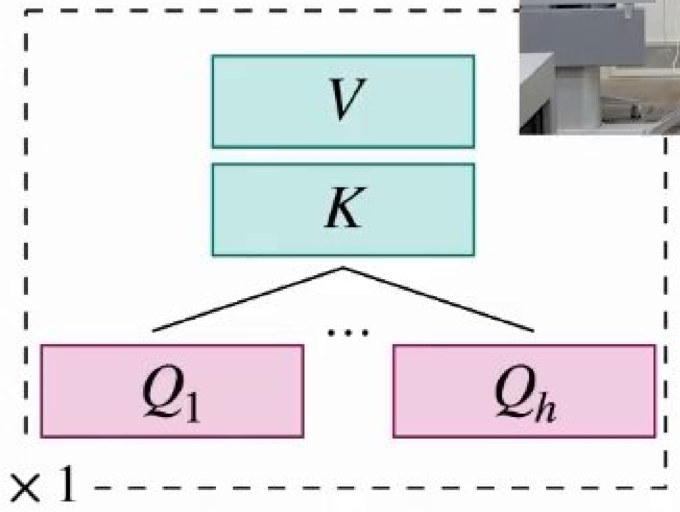
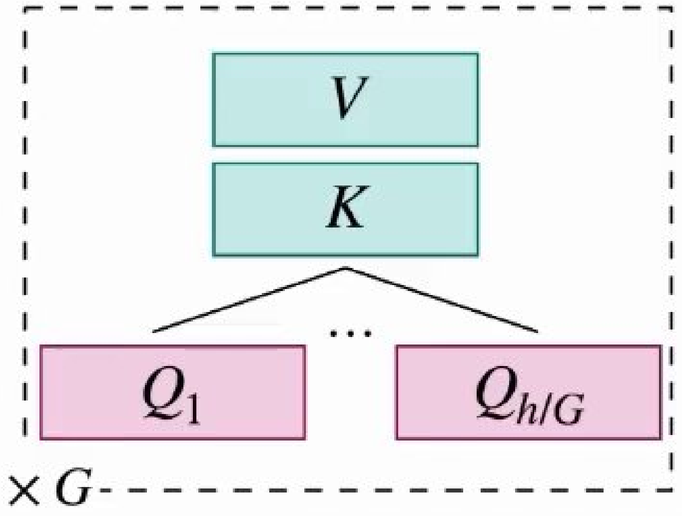
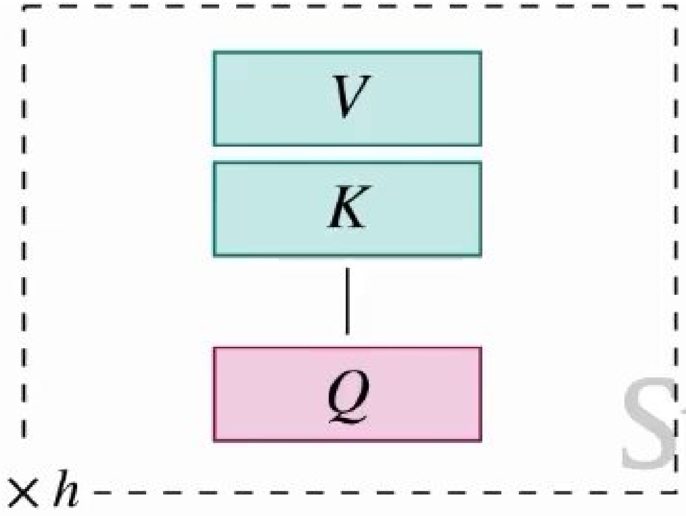
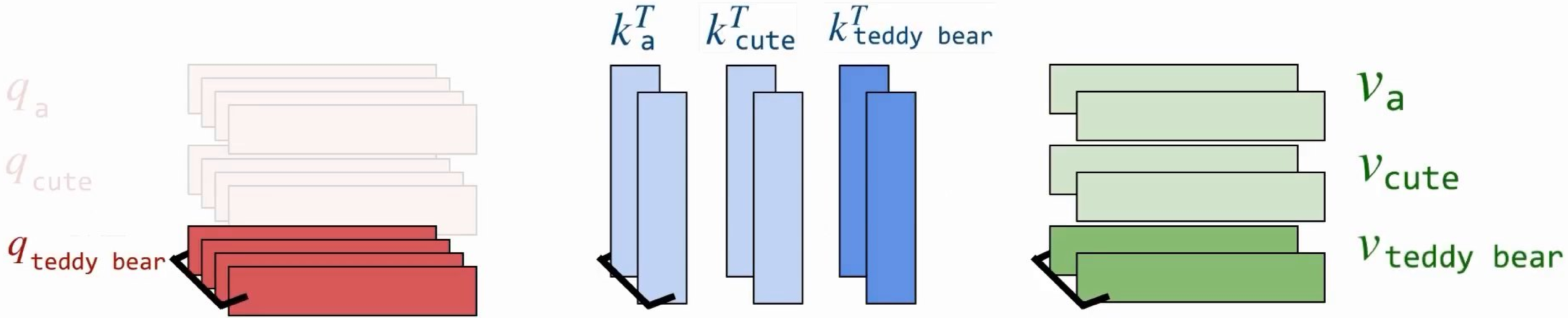
$G = 1$	**M**ulti-**Q**uery **A**ttention (MQA)	
$1 < G < h$	**G**roup-**Q**uery **A**ttention (GQA)	
$G = h$	**M**ulti-**H**ead **A**ttention (MHA)	

Figure from "Super Study Guide: Transformers & Large Language Models", Amidi et al., 2024.

Sharing attention heads with GQA



Number of **query heads**	Number of **key heads**	Number of **value heads**
= h	= G < h	= G < h

Manage memory with PagedAttention

Observation. Lots of memory waste when storing KV cache.

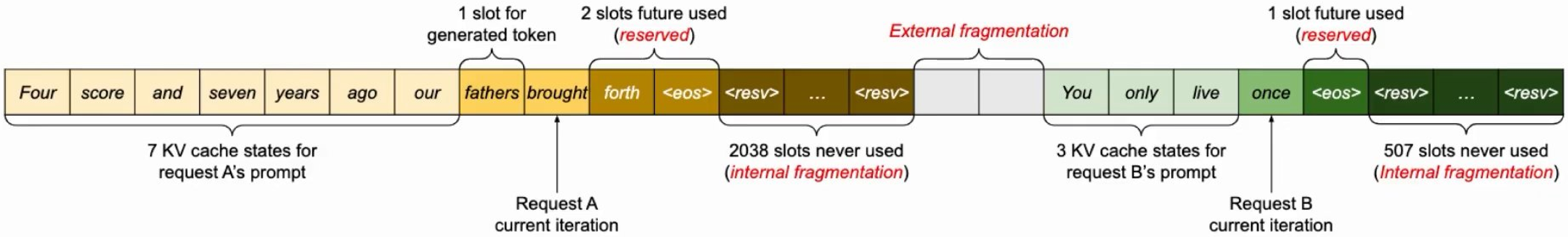


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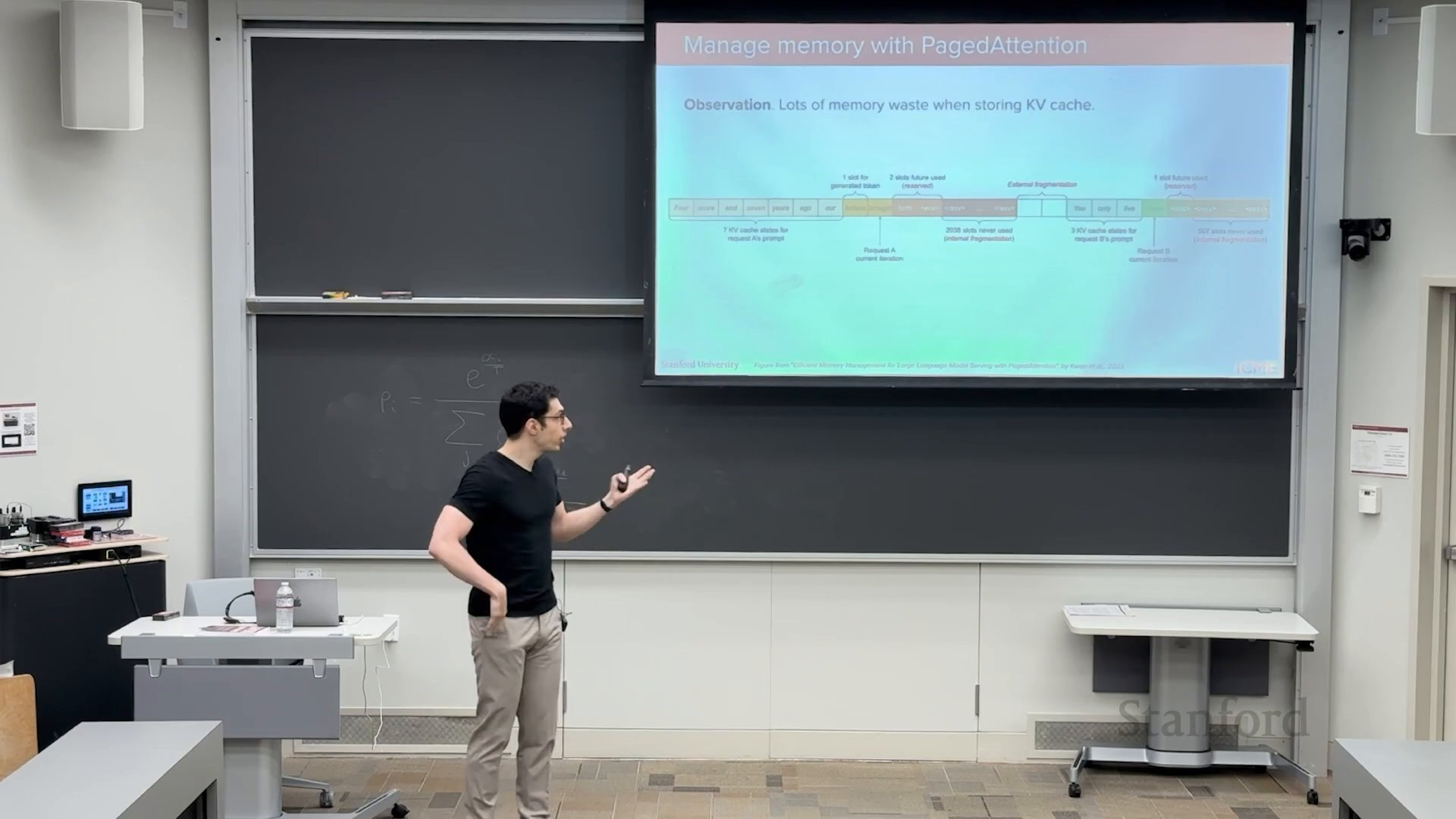
Figure from "Efficient Memory Management for Large Language Model Serving with PagedAttention", by Kwon et al., 2023.



Manage memory with PagedAttention
Observation. Lots of memory waste when storing KV cache.
1 slot for generated token
2 slots future used (reserved)
External fragmentation
1 slot future used (reserved)
Four
score
and
seven
years
ago
our
You
only
live
7 KV cache states for request A's prompt
Request A current iteration
2038 slots never used (internal fragmentation)
3 KV cache states for request B's prompt
Request B current iteration
507 slots never used (internal fragmentation)
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Manage memory with PagedAttention

Observation. Lots of memory waste when storing KV cache.

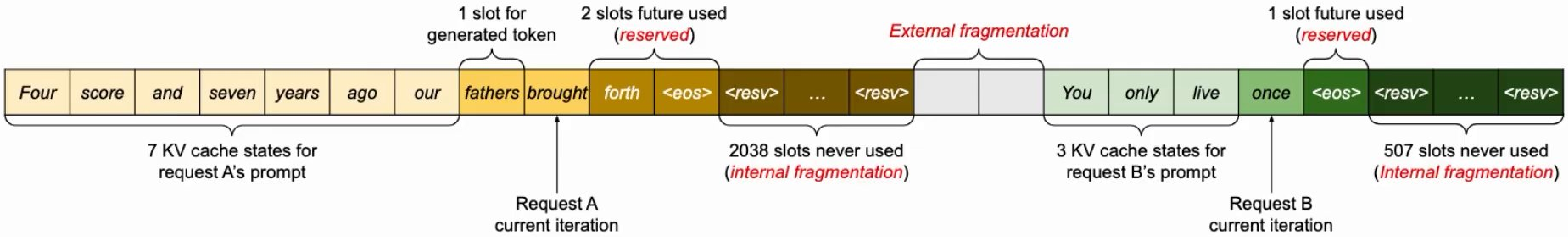

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Figure from "Efficient Memory Management for Large Language Model Serving with PagedAttention", by Kwon et al., 2023.

Manage memory with PagedAttention

Idea. Store K and V in non-contiguous space to minimize wasted memory.

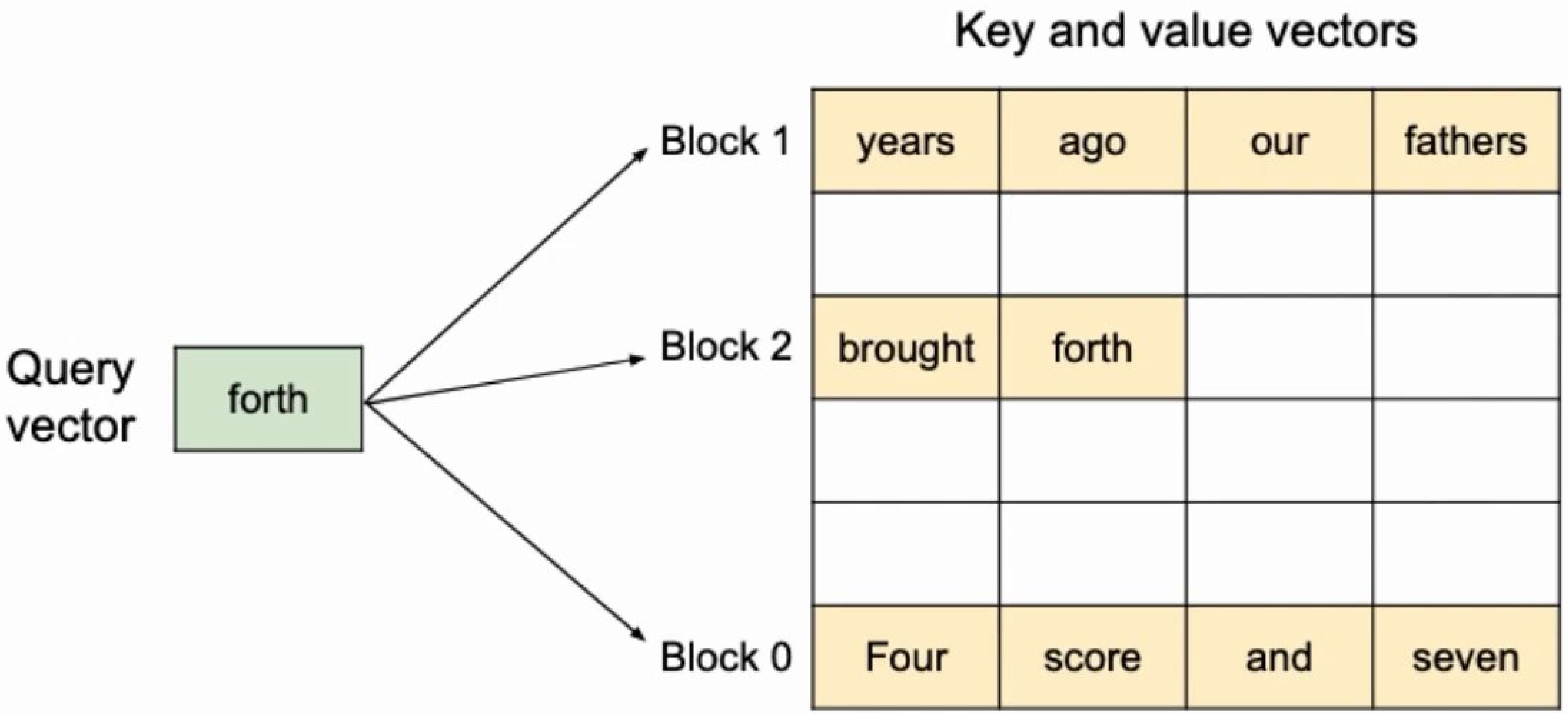

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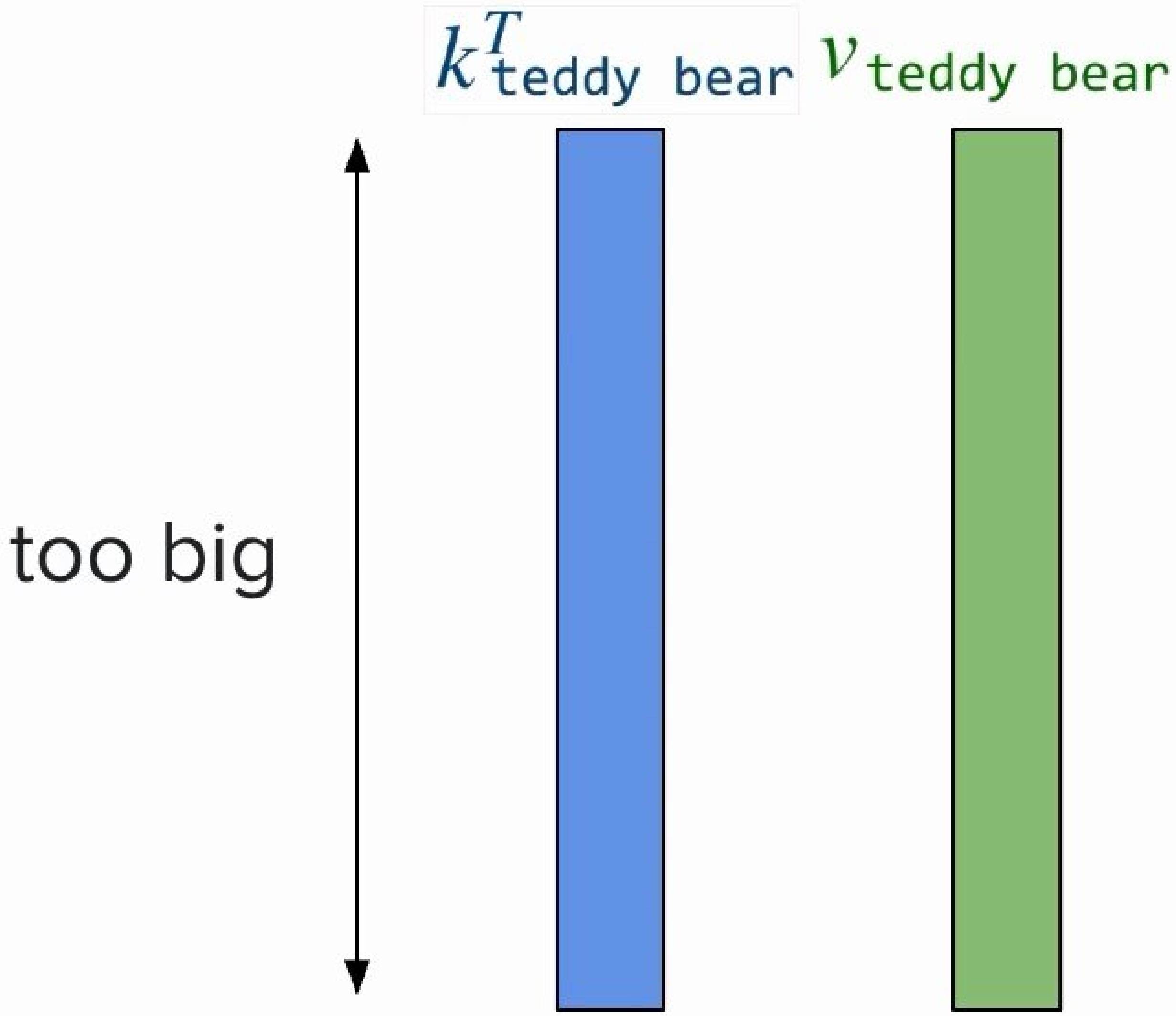
Figure from "Efficient Memory Management for Large Language Model Serving with PagedAttention", by Kwon et al., 2023.

Reduce memory of KV cache with latent a

Goal. Reduce dimension of K and V stored in memory.



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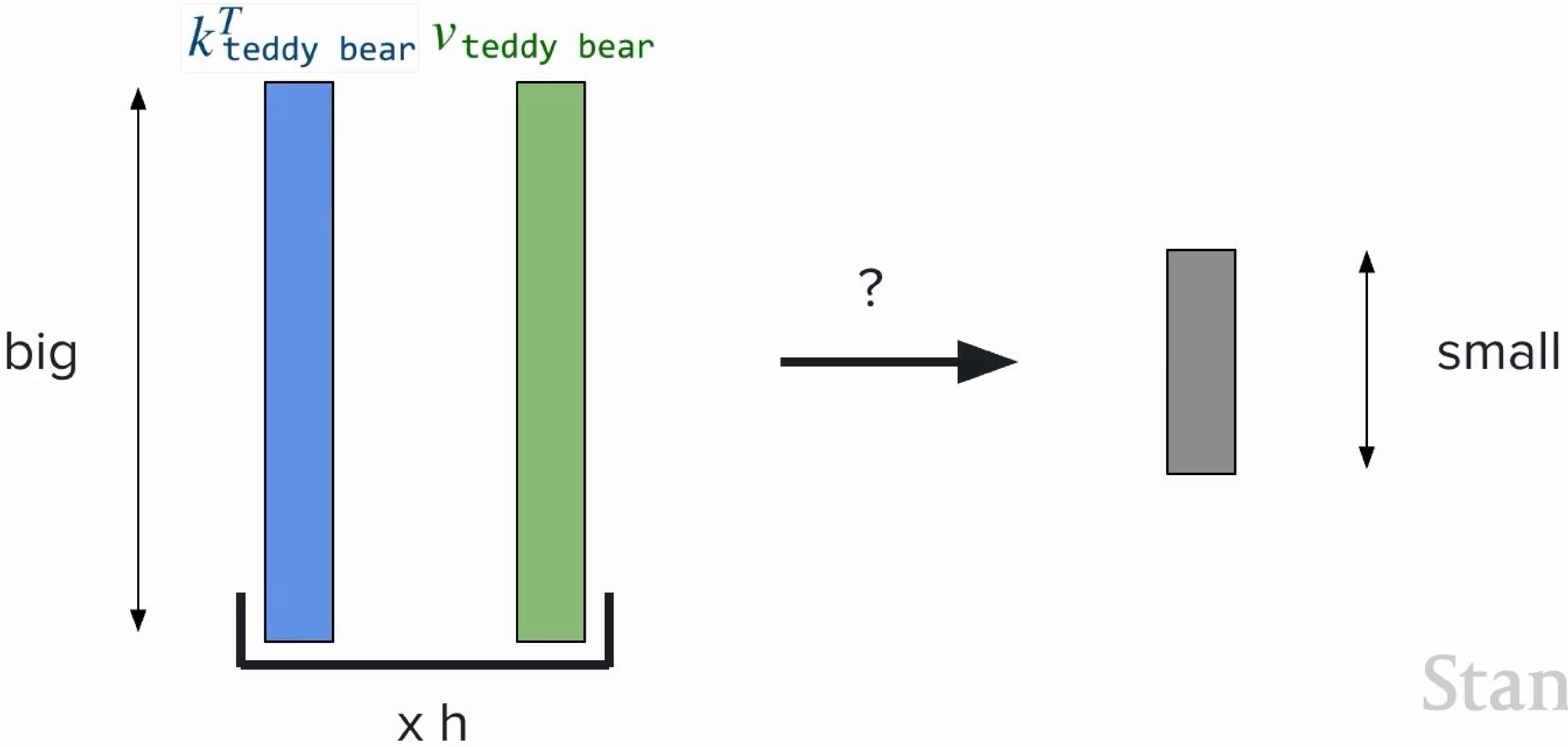
Reduce memory of KV cache with latent a

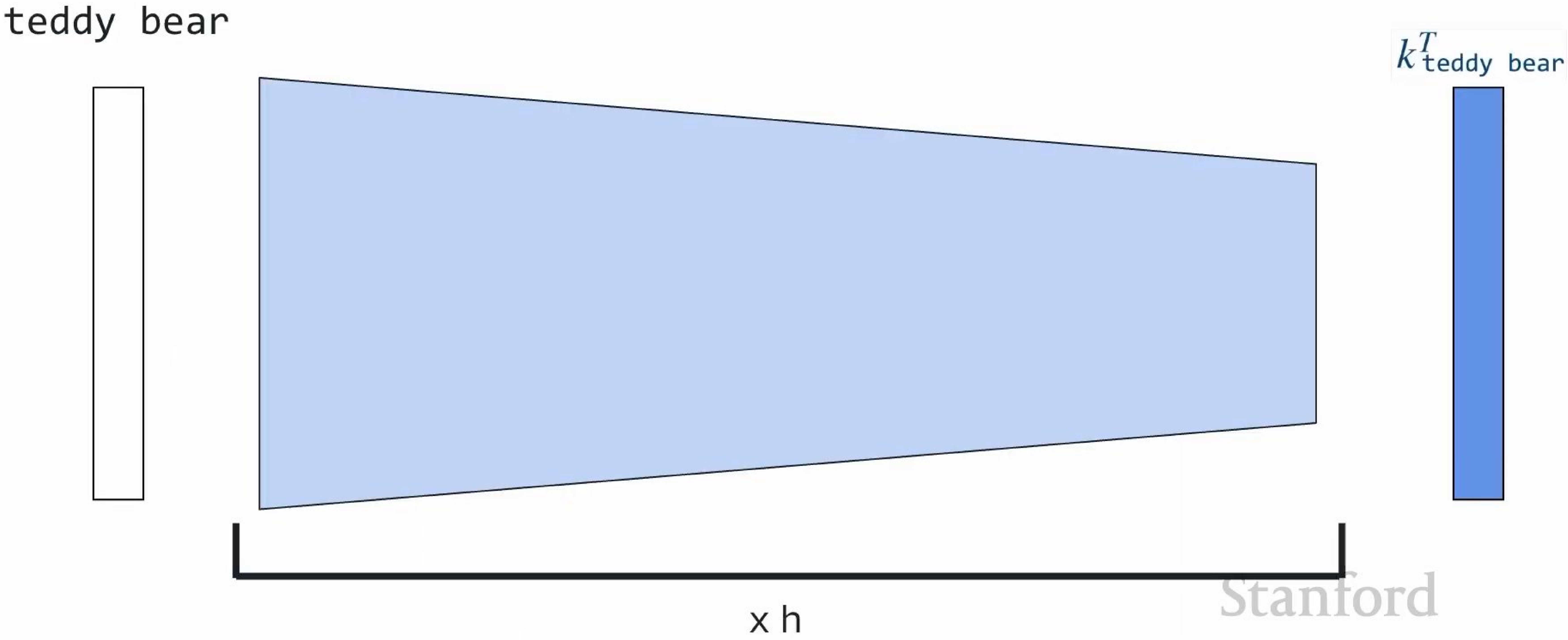
Solution. Store compressed representations instead!



"*DeepSeek-V2: A Strong, Economical, and Efficient Mixture-of-Experts Language Model*", by DeepSeek, 2023.

Reduce memory of KV cache with latent a

BEFORE



Token generation tricks
Output
Probabilities
Softmax
Linear
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Speeding up decoding with speculative c

Idea. Use a draft (small) model to generate tokens validated by a target (big) model.

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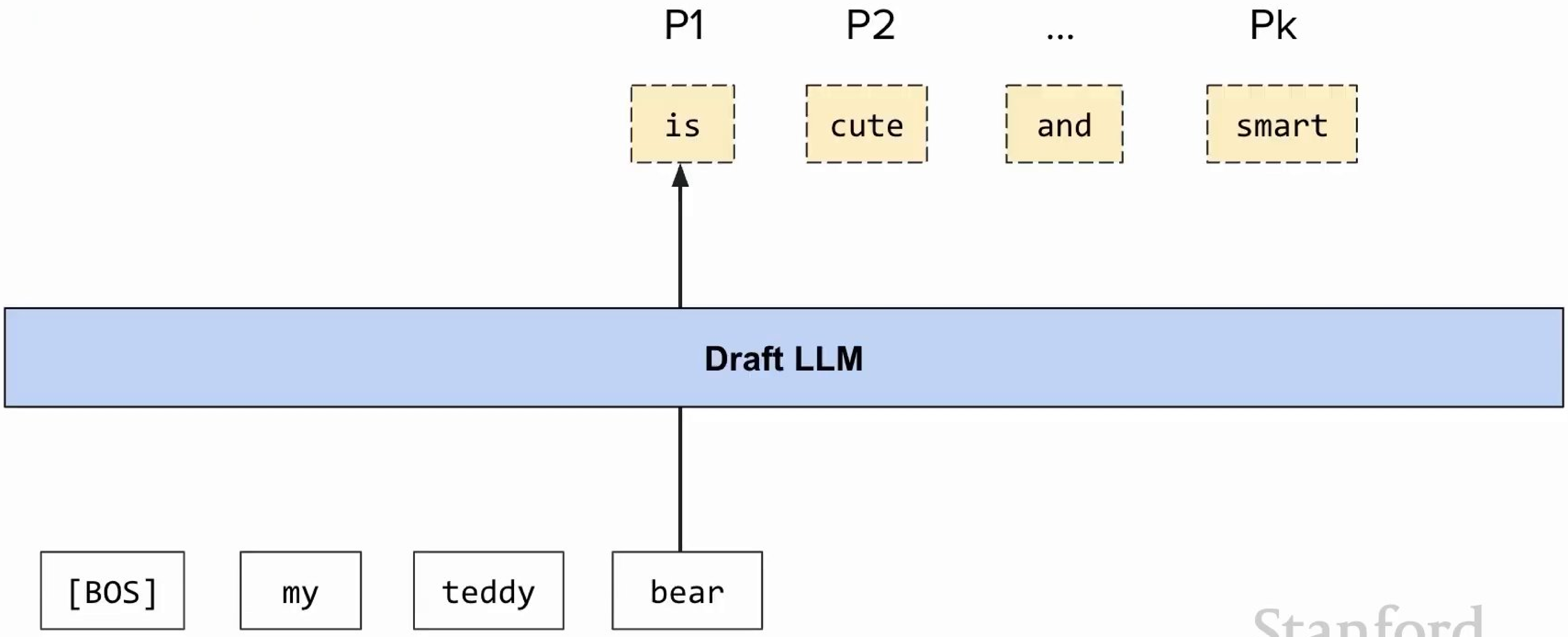
Speeding up decoding with speculative d



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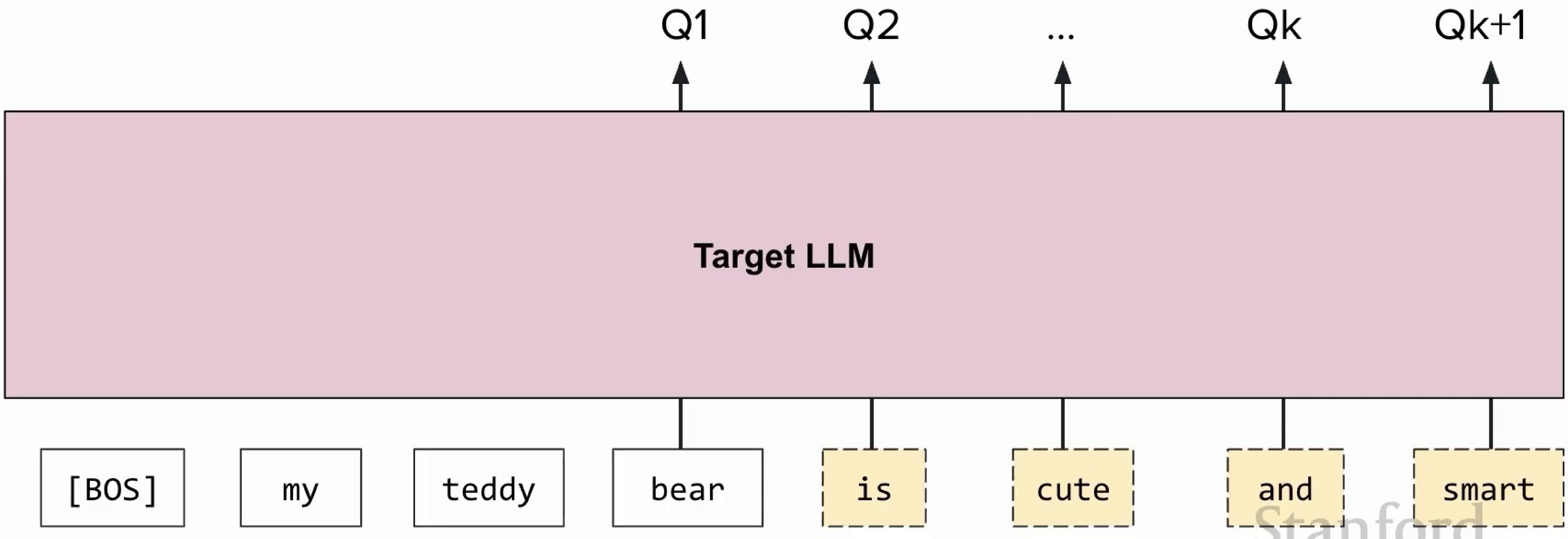
"*Accelerating Large Language Model Decoding with Speculative Sampling*", Chen et al., 2023.

Speeding up decoding with speculative d



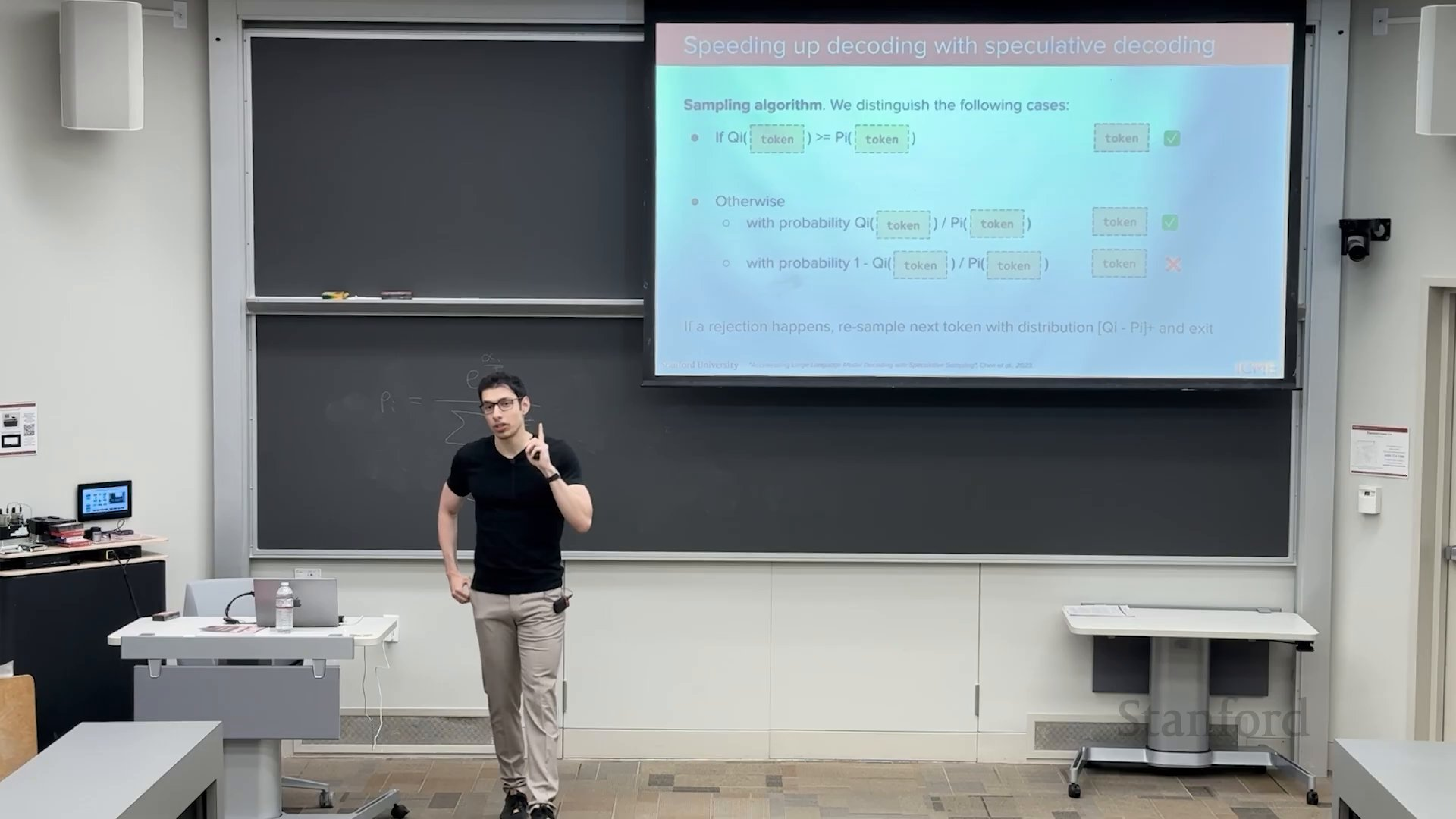
 "Accelerating Large Language Model Decoding with Speculative Sampling", Chen et al., 2023.

Speeding up decoding with speculative d

Sampling algorithm. We distinguish the following cases:

- If Qi(token) >= Pi(token) token ✅
- Otherwise
  - with probability Qi(token) / Pi(token) token ✅
  - with probability 1 - Qi(token) / Pi(token) token ❌

If a rejection happens, re-sample next token with distribution [Qi - Pi]+ and exit


Speeding up decoding with speculative decoding
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Speeding up decoding with speculative d

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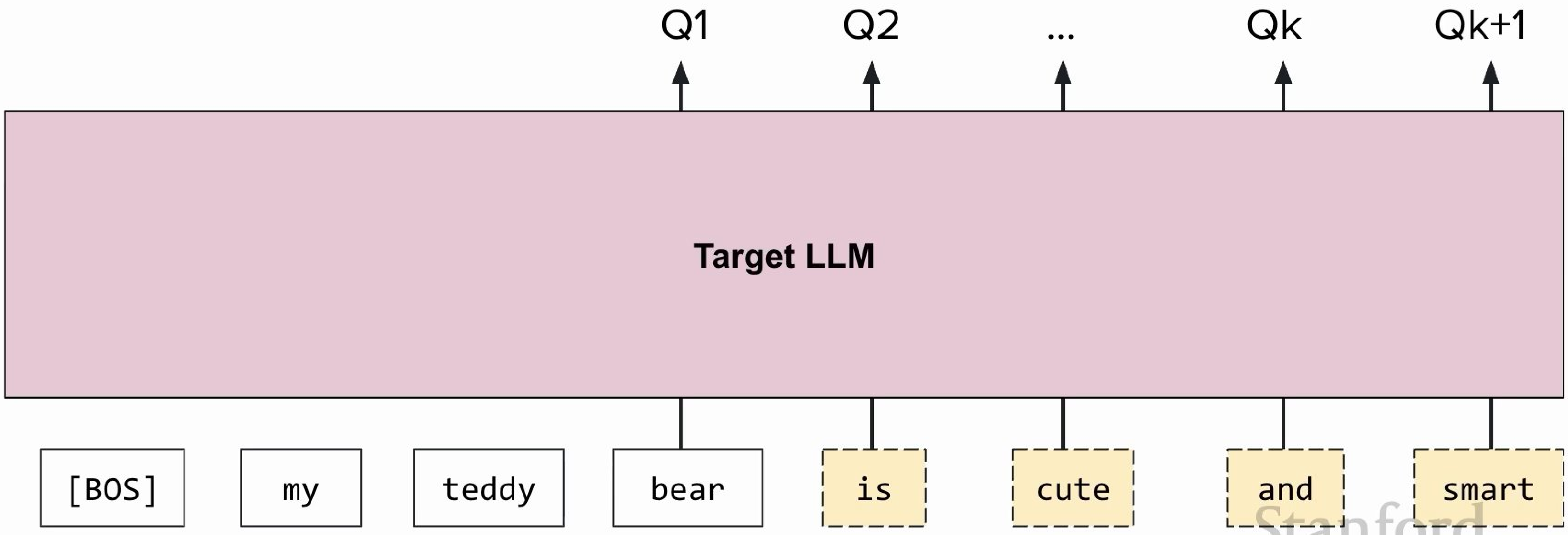
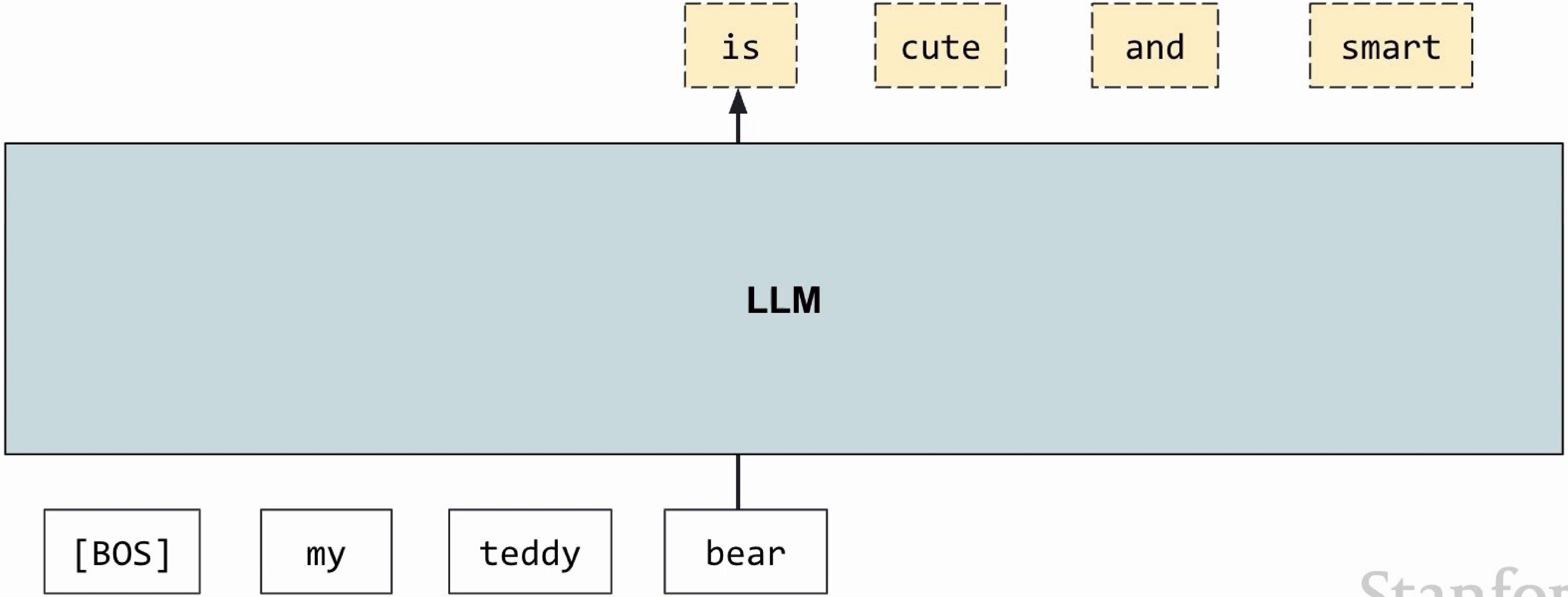
Speeding up decoding with speculative d



Generate several tokens at once via MTP

MTP = **M**ulti-**T**oken **P**rediction



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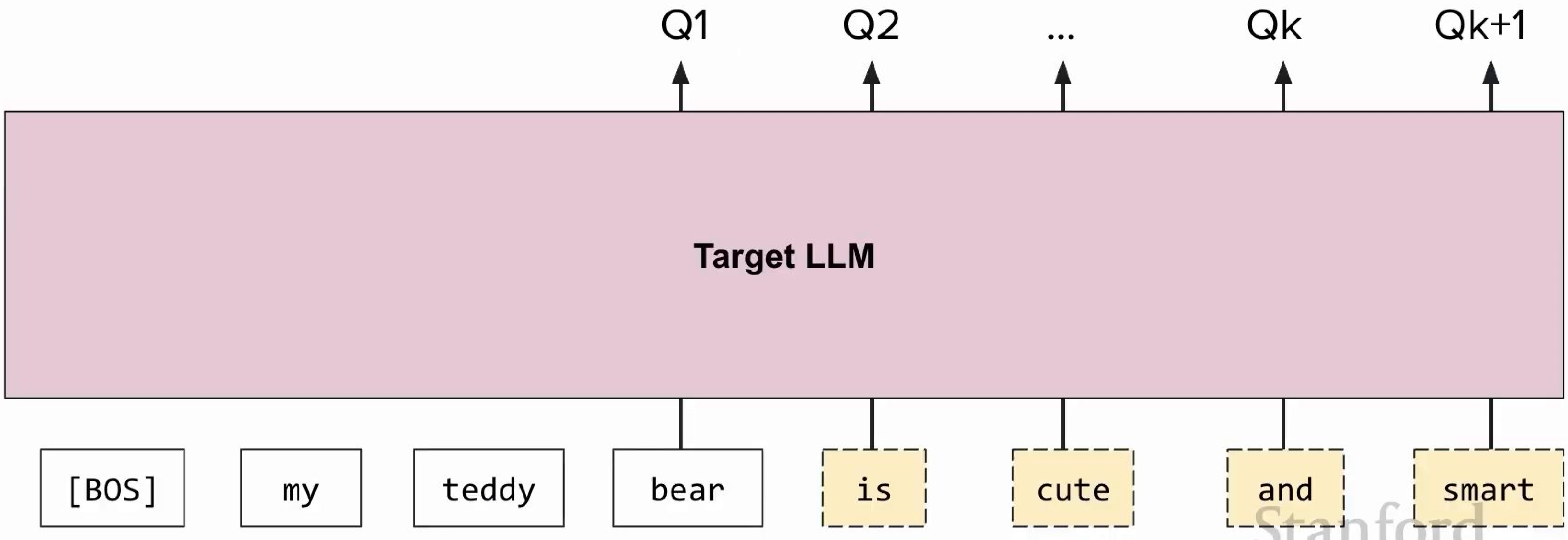
"*Better & Faster Large Language Models via Multi-token Prediction*", *Gloeckle et al., 2024.*

Speeding up decoding with speculative d



"*Accelerating Large Language Model Decoding with Speculative Sampling*", Chen et al., 2023.

Generate several tokens at once via MTP

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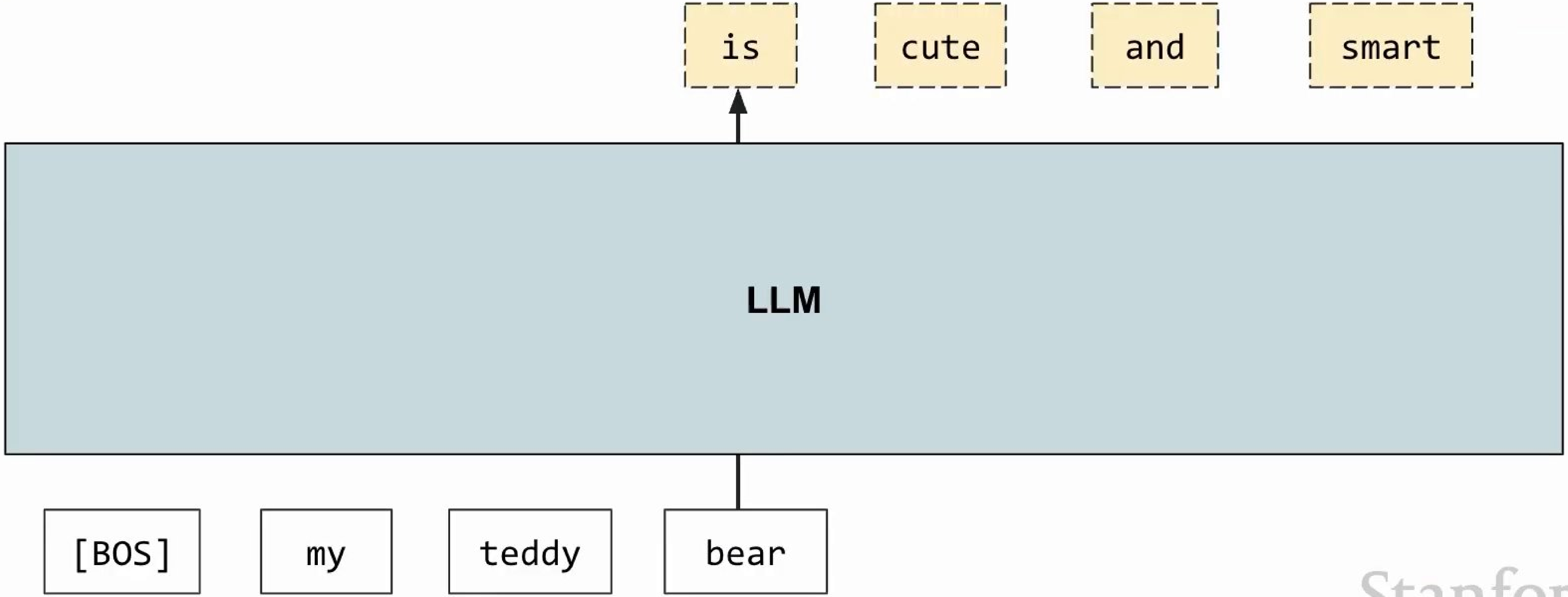

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Generate several tokens at once via MTP

Idea. Train k prediction heads: same draft and target models!

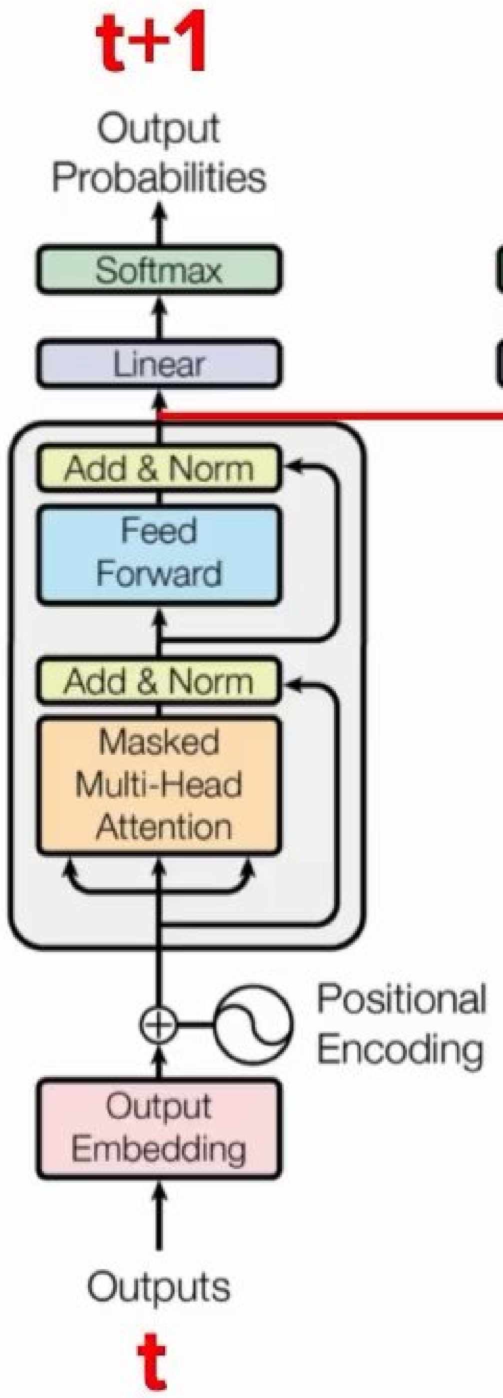

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Figure adapted from "Attention is All You Need", Vaswani et al., 2017.

Challenges

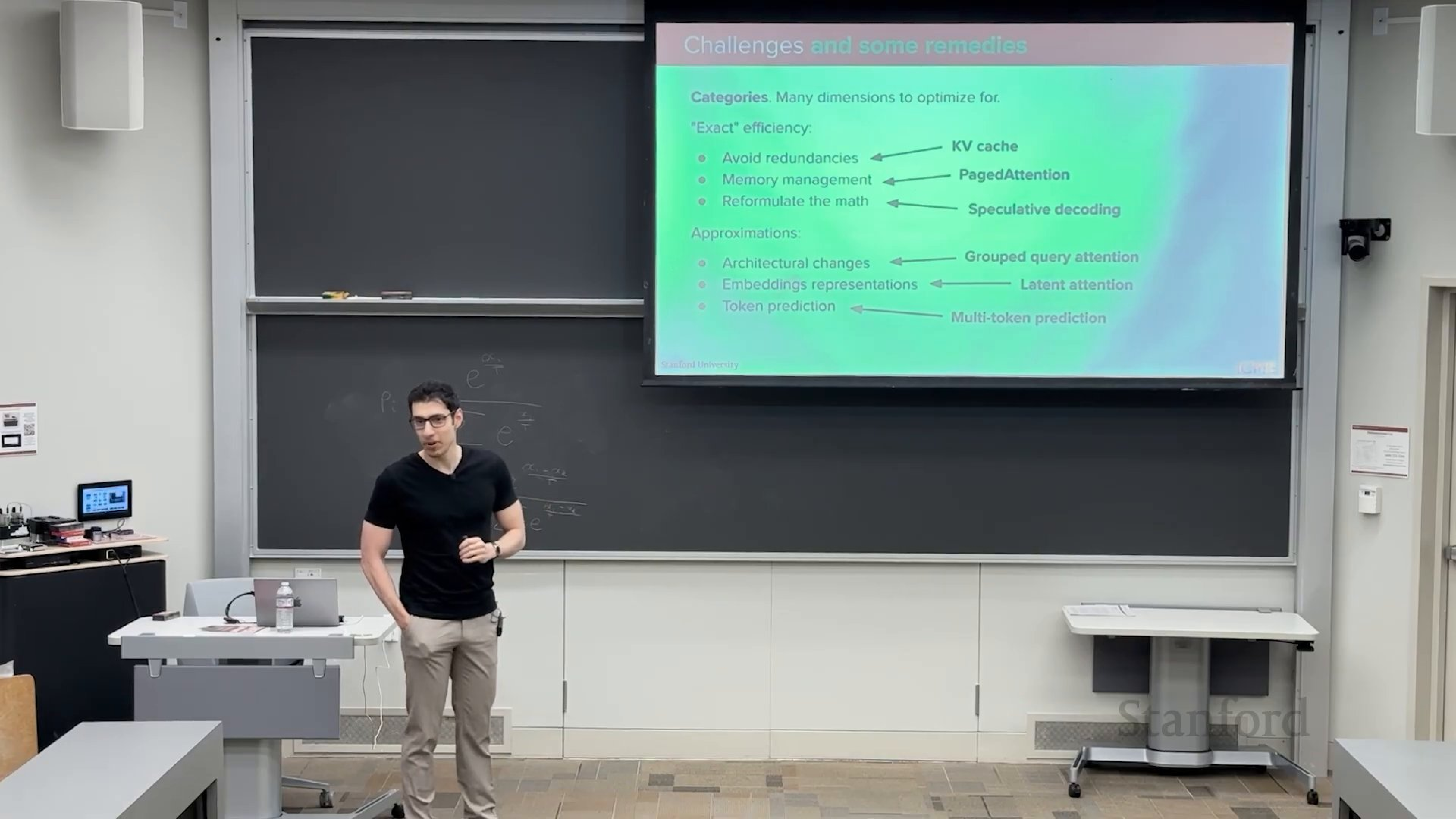
Categories. Many dimensions to optimize for.

"Exact" efficiency:

- Avoid redundancies
- Memory management
- Reformulate the math

Approximations:

- Architectural changes
- Embeddings representations
- Token prediction


Challenges and some remedies
Categories. Many dimensions to optimize for.
"Exact" efficiency:
Avoid redundancies
KV cache
Memory management
PagedAttention
Reformulate the math
Speculative decoding
Approximations:
Architectural changes
Grouped query attention
Embeddings representations
Latent attention
Token prediction
Multi-token prediction
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