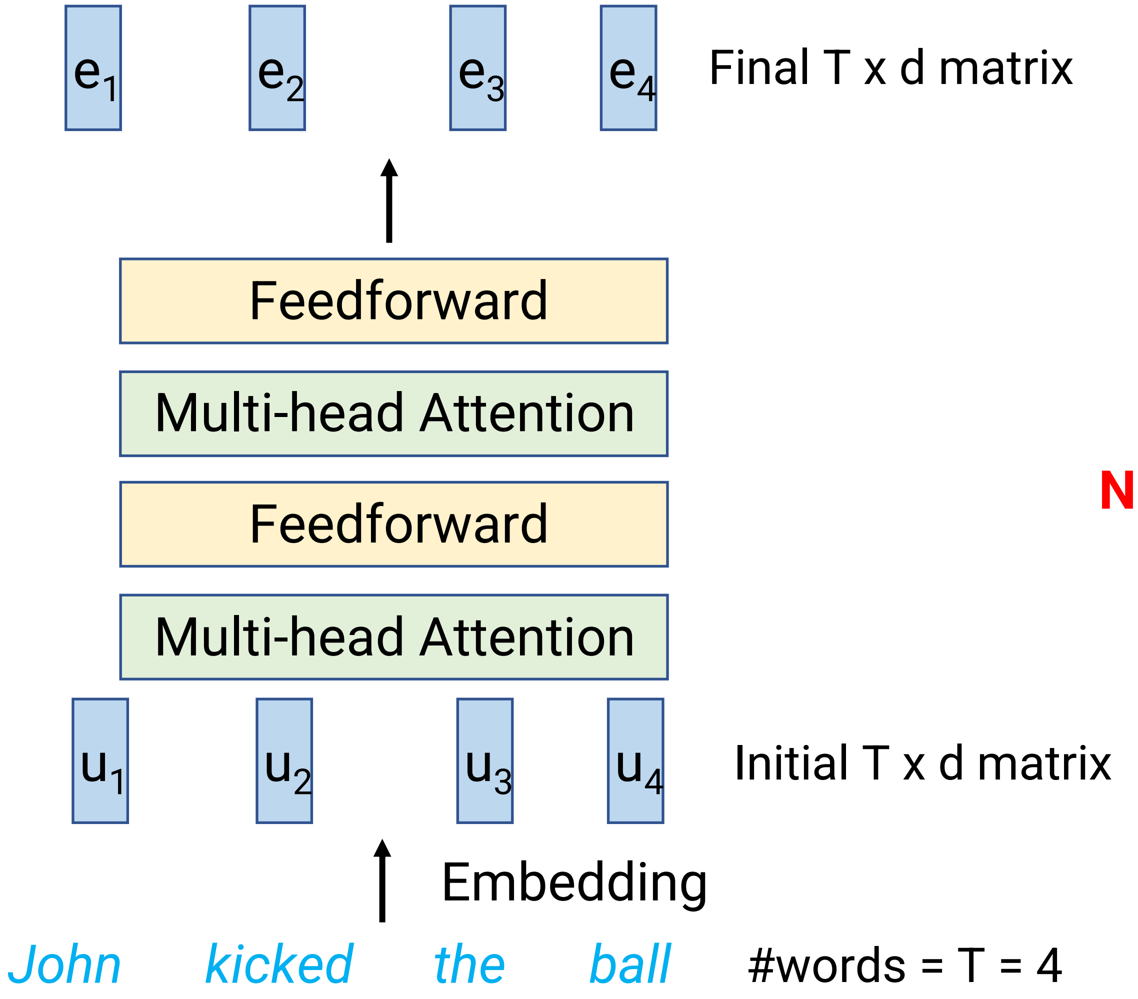
Transformers II, Pretraining

Robin Jia
USC CSCI 467, Spring 2025
March 27, 2025

Review: Transformer at a high level

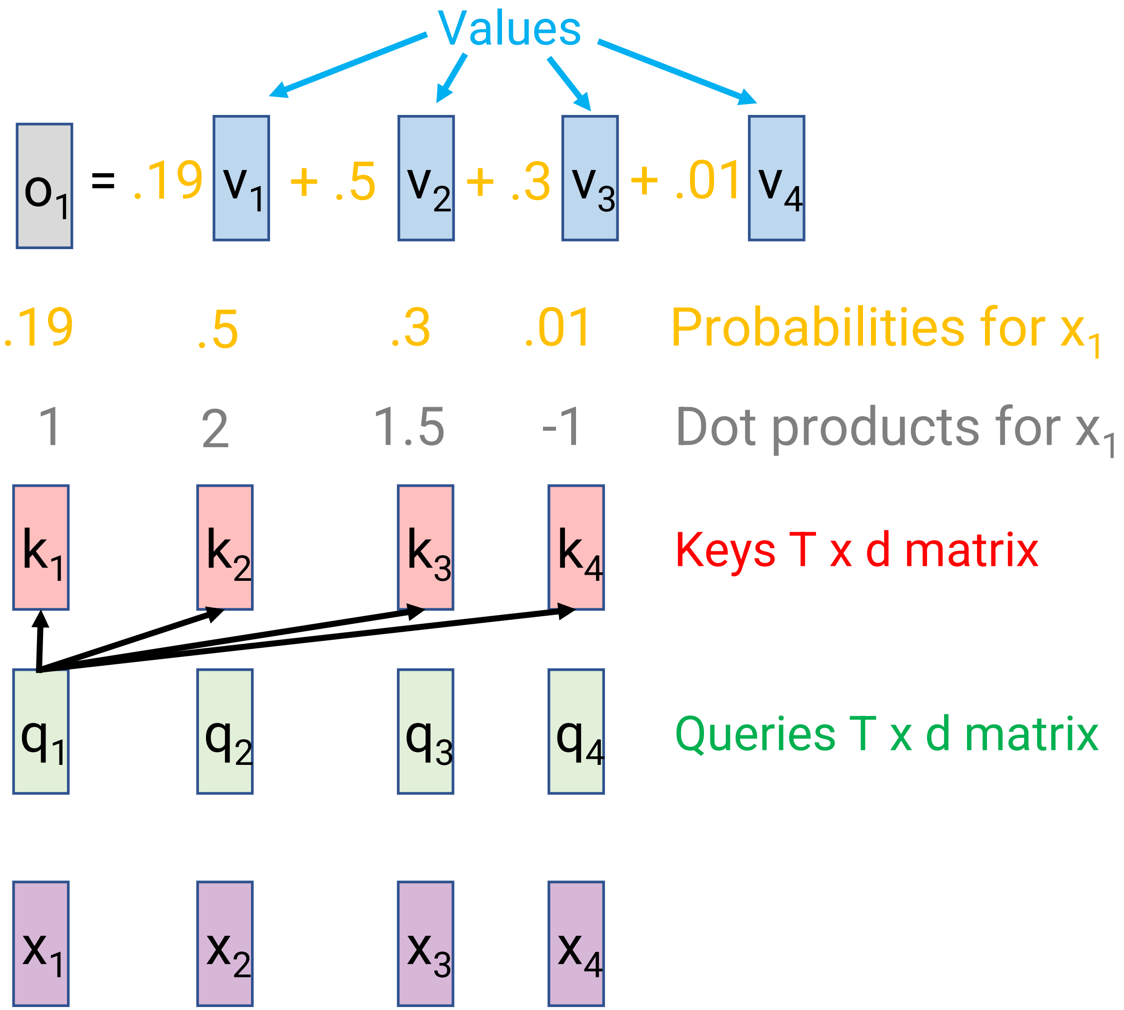


- One transformer consists of
  - Initial embeddings for each word of size d
    - Let T =#words, so initially we have a T x d matrix
  - Alternating layers of
    - **"Multi-headed" attention layer**
    - Feedforward layer
    - Both take in T x d matrix and output a new T x d matrix
  - Plus some bells and whistles…

New!

Familiar

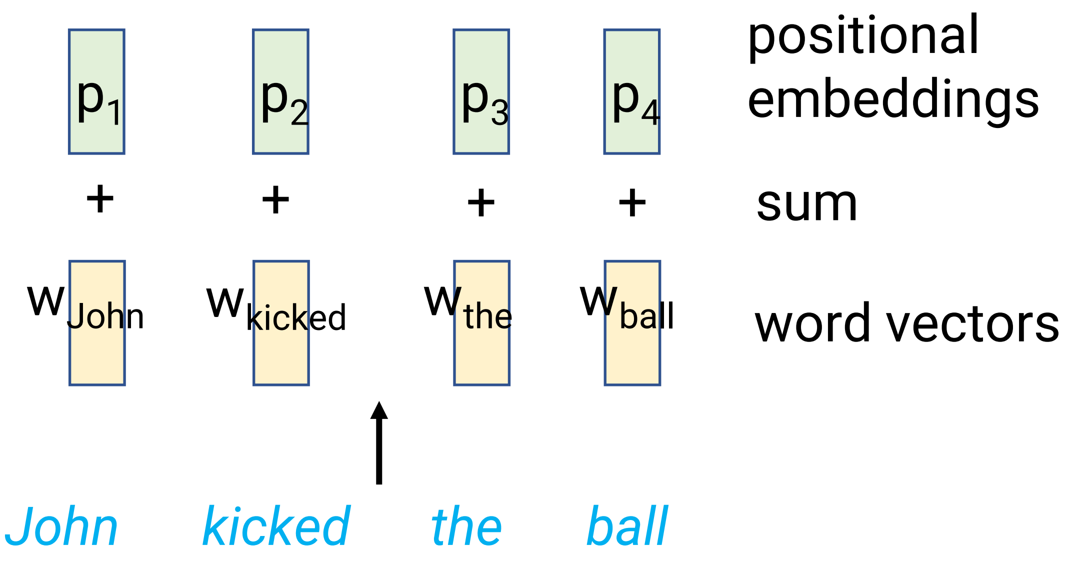
Review: Multi-headed Attention



- Input: T vectors $x_1, \ldots, x_T$ each of dimension d
- Apply 3 separate linear layers to each x_t:
  - Query vectors $q_t = W^Q * x_t$
  - Keys vectors $k_t = W^K * x_t$
  - Value vectors $v_t = W^V * x_t$
- To compute output o_t:
  - Dot product q_t with each key vector k_i
  - Apply softmax to get probabilities p_i
  - Compute $o_t = \sum_{i=1}^{T} p_i * v_i$
- Have n heads with n different sets of parameters, then concatenate results
  - Choose $d_{attn} = d/n$ so output is also dimension d
- Parameters W^Q, W^K, W^V for each head must be learned by gradient descent

Review: Initial embedding layer

- As before, learn a vector for each word in vocabulary
- Is this enough?
  - Both attention and feedforward layers are **order invariant**
  - Need the initial embeddings to also encode order of words!
- Solution: **Positional embeddings**
  - Learn a different vector for each index
  - Gets added to word vector at that index



RNNs vs. Transformers (Encoders)

RNNs

- Process a sentence **one word at a time**
- Each "step" of computation is reading **one more word** (time dimension)
- Each hidden state encodes **information about sentence up to the current word**

Both

- Input = sequence of vectors, representing words
- Output = sequence of hidden state vectors, one for each input word

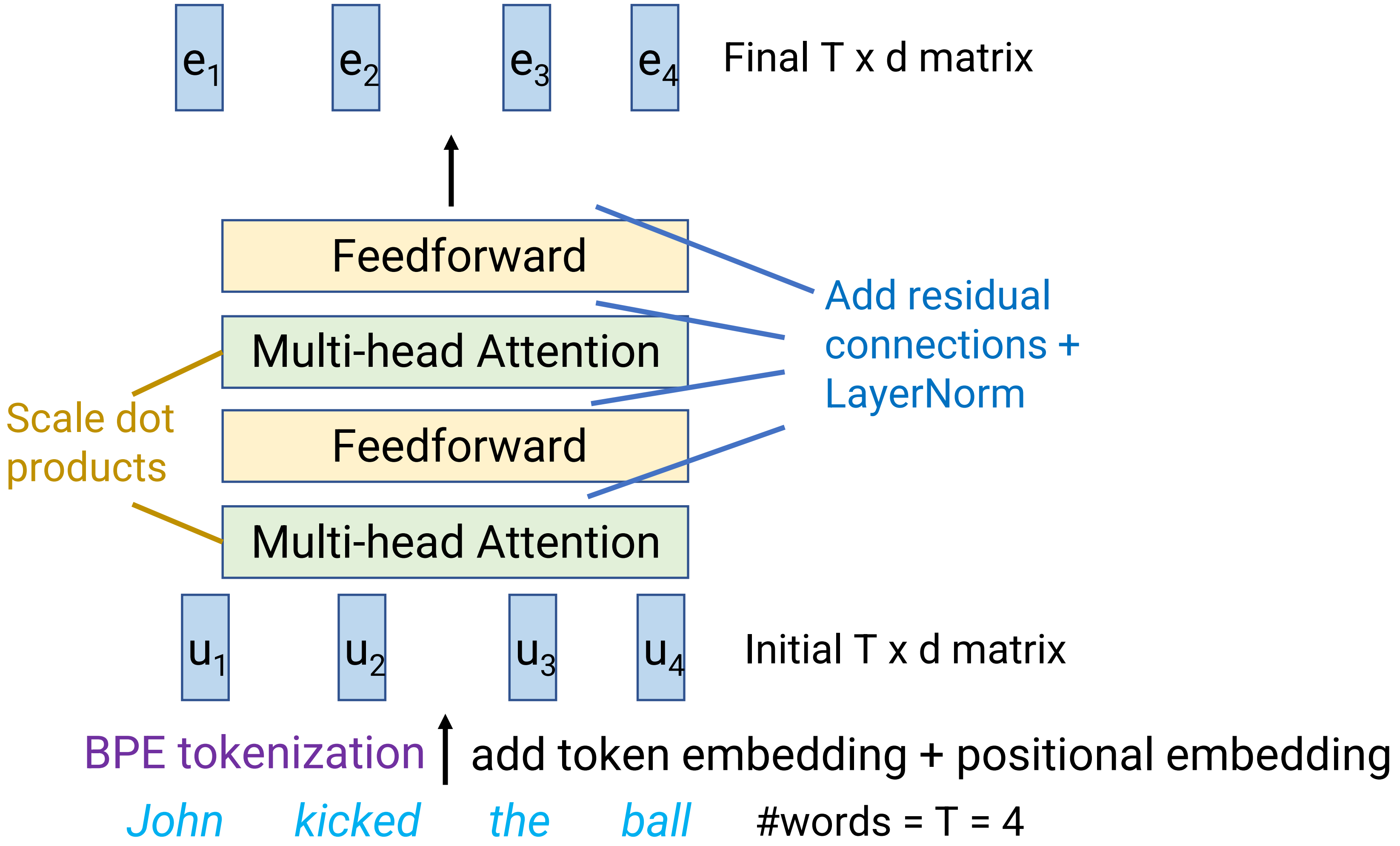
Transformers

- Process **all words of the sentence at the same time** (in parallel)
- Each "step" of computation is applying **one more layer** (depth dimension; more like a CNN)
- Each hidden state encodes **information about that word in the context of the whole sentence**

Today's Plan

- Transformers in full detail
- Pre-training
- Transformer decoders
- Vision Transformers

The Full Transformer



Full Transformer also includes bells and whistles:

- Byte pair encoding
- Scaled dot product attention
- Residual connections between layers
- LayerNorm

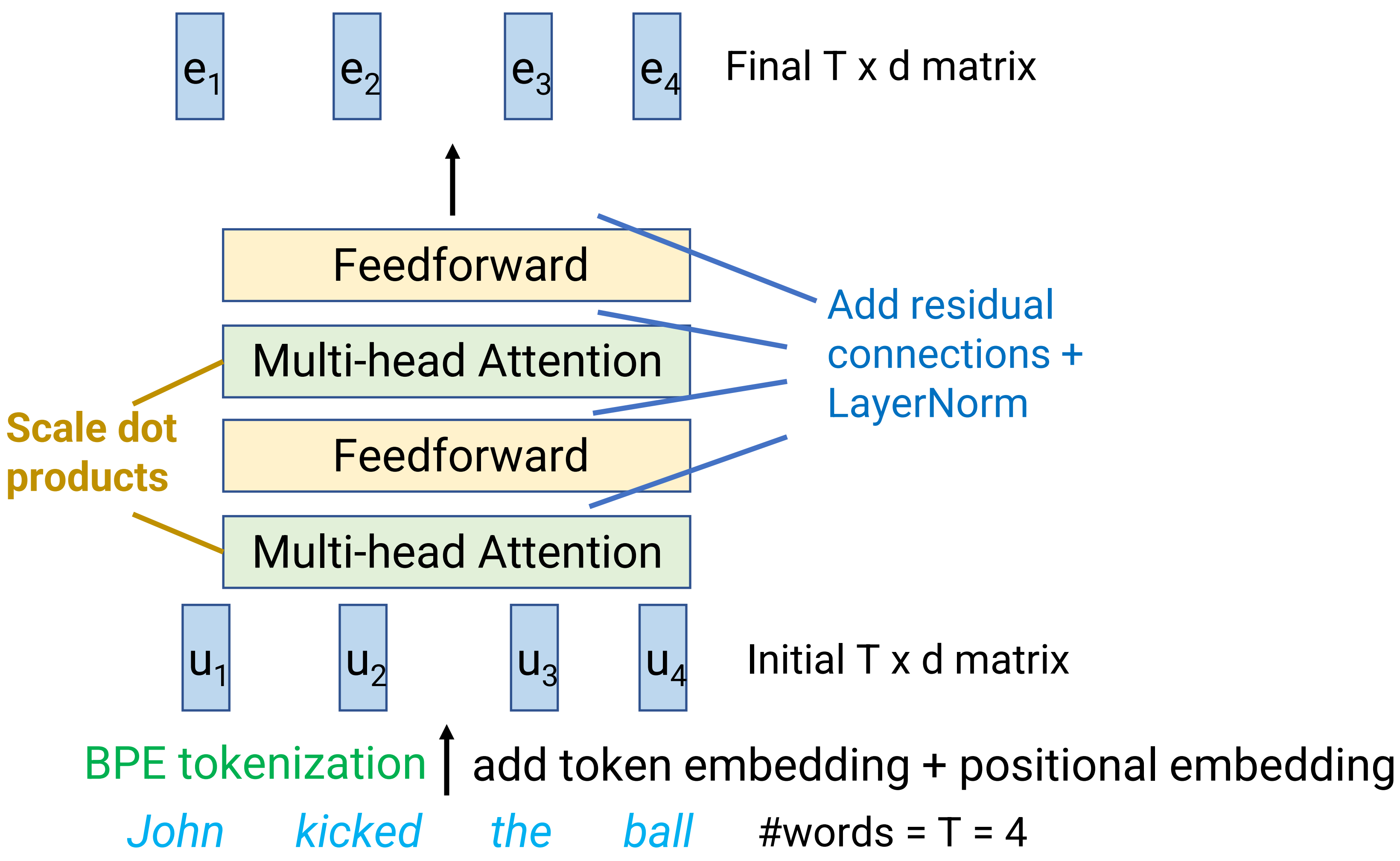
Byte Pair Encoding

- Normal word vectors have a problem: How to deal with super rare words?
  - Names? Typos?
  - Vocabulary can’t contain literally every possible word…
- Solution: Tokenize string into “subword tokens”
  - Common words = 1 token
  - Rare words = multiple tokens

Aragorn told Frodo to mind Lothlorien — 6 words

'Ar', 'ag', 'orn', ‘ told', ‘ Fro', 'do’, ‘ to', ‘ mind’, ‘ L', 'oth', 'lor', 'ien' — 12 subword tokens

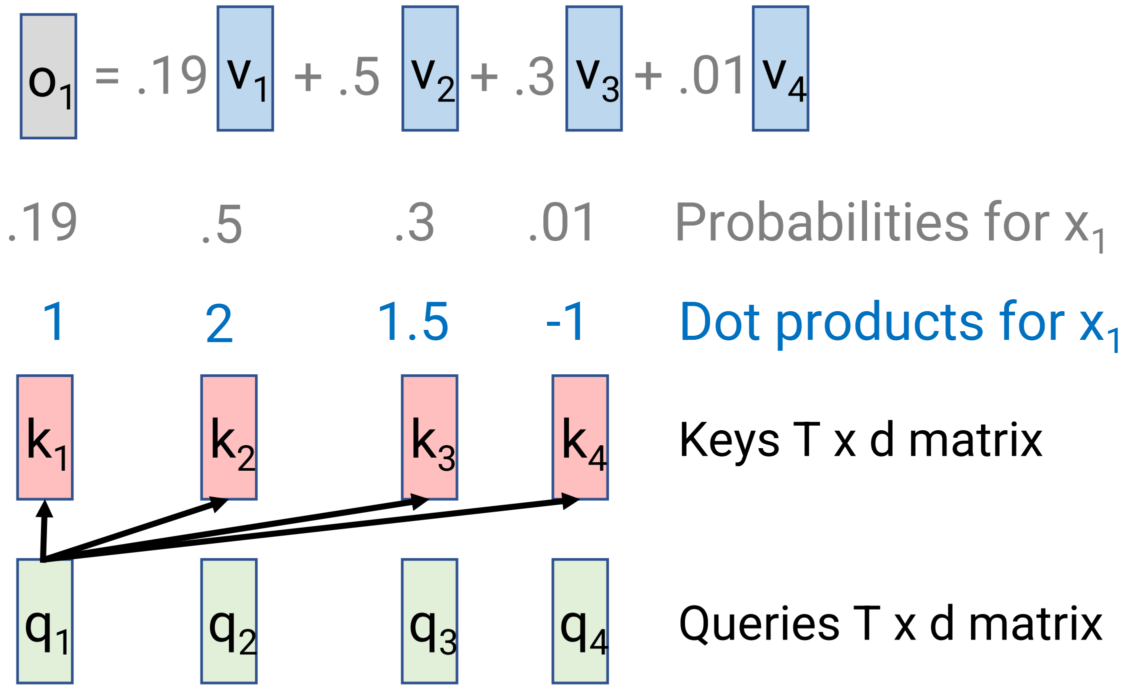
The Full Transformer



Full Transformer also includes bells and whistles:

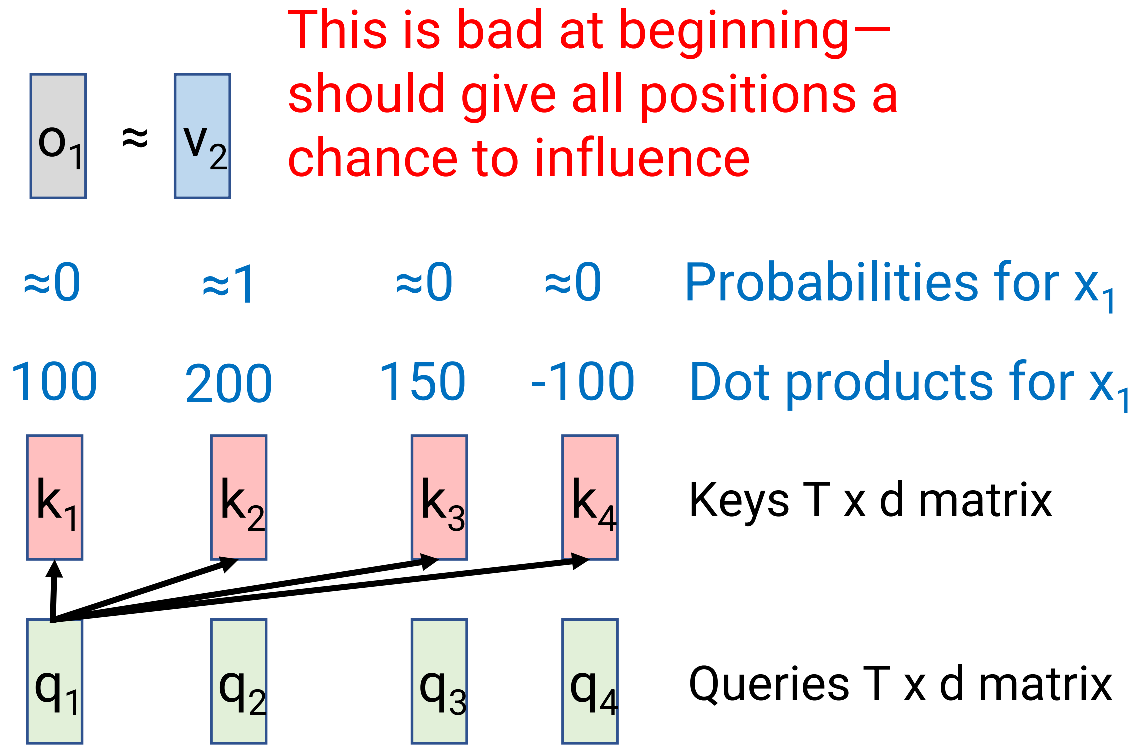
- Byte pair encoding
- **Scaled dot product attention**
- Residual connections between layers
- LayerNorm

Scaled dot product attention



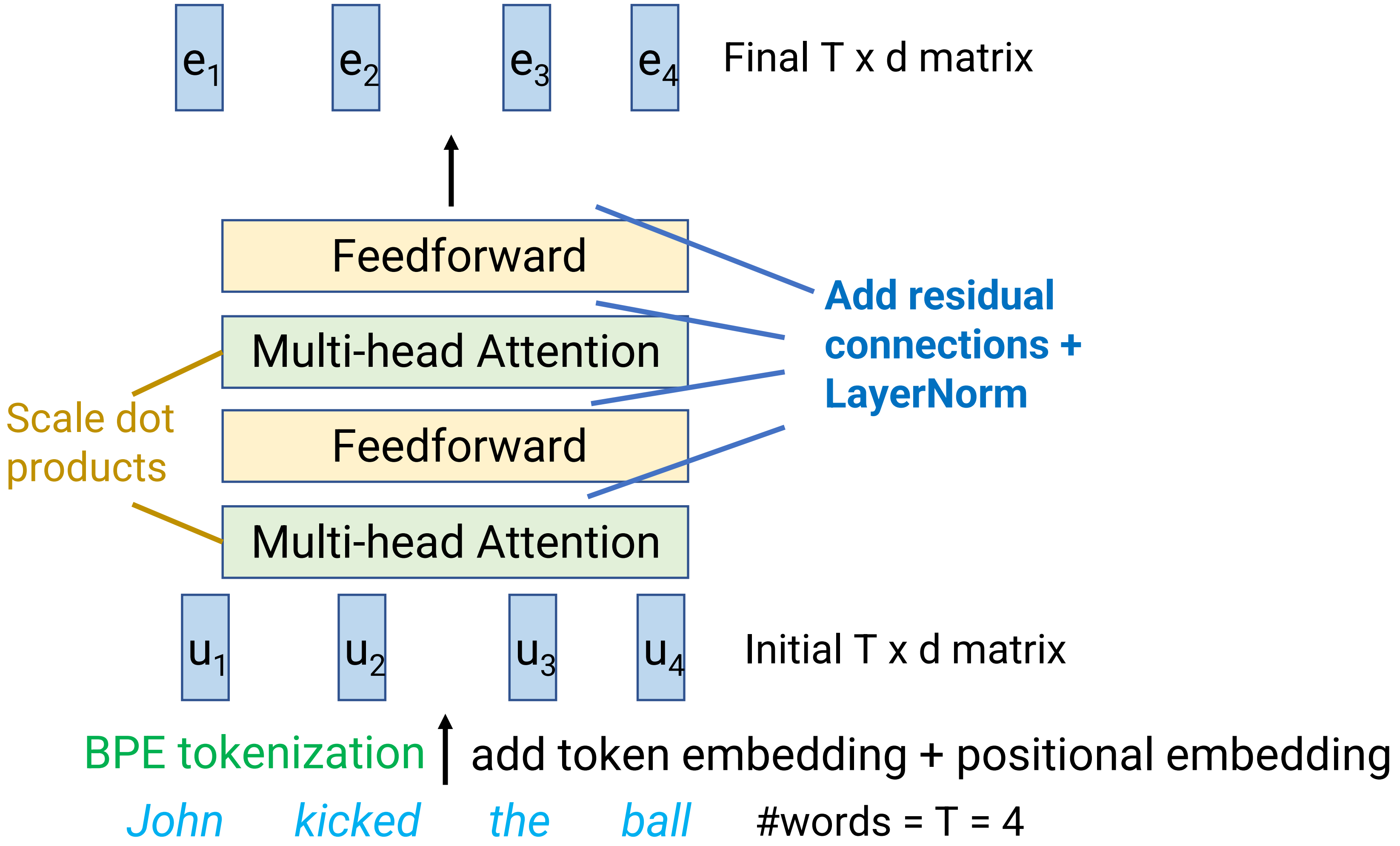
- Earlier I said, "Dot product q_1 with $[k_1, \ldots, k_T]$"
- Actually, you take dot product and then divide by $\sqrt{d_{attn}}$
- Why?
  - If d large, dot product between random vectors will be large
  - This makes probabilities close to 0/1
  - Scaling dot products down encourages more even attention at beginning

Scaled dot product attention



- Earlier I said, "Dot product q_1 with $[k_1, \ldots, k_T]$"
- Actually, you take dot product and then divide by $\sqrt{d_{attn}}$
- Why?
  - If d large, dot product between random vectors will be large
  - This makes probabilities close to 0/1
  - Scaling dot products down encourages more even attention at beginning

The Full Transformer

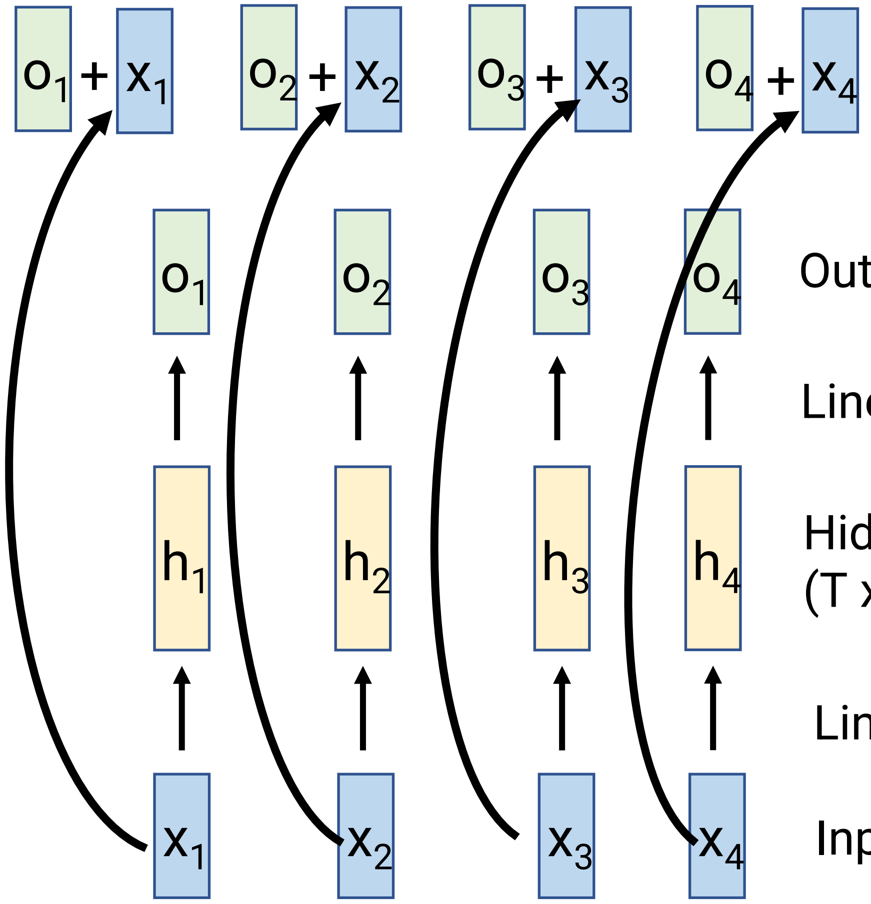


Full Transformer also includes bells and whistles:

- Byte pair encoding
- Scaled dot product attention
- **Residual connections between layers**
- **LayerNorm**

Residual Connections

- Feedforward and multi-headed attention layers
  - Take in T x d matrix X
  - Output T x d matrix O
- We add a "residual" connection: we actually use X + O as output
  - Makes it easy to copy information from input to output
  - Think of O as how much we **change** the previous value
- Same idea also common in CNNs!
  - Reduces vanishing gradient issues



Layer Normalization ("LayerNorm")

- LayerNorm is a layer/building block that "normalizes" a vector
- Input x: vector of size d
- Output y: vector of size d
- Formula: $$\mu = \frac{1}{d}\sum_{i=1}^{d} x_i$$ Mean of components of x

$$\sigma^2 = \frac{1}{d}\sum_{i=1}^{d}(x_i - \mu)^2$$ Variance of components of x

$$y = a \odot \underbrace{\boxed{\frac{x-\mu}{\sqrt{\sigma^2+\varepsilon}}}}_{\text{Normalized x}} + b$$

1. Normalize: Subtract by mean, divide by standard deviation
2. Rescale: Elementwise multiply by a, add b

- Parameters
  - a & b are vector parameters, let model learn good scale/shift per dimension
    - Without these, all vectors forced to have mean=0, variance=1
  - ε is hyperparameter: Some small number to prevent division by 0

x = [100, 200, 100, 0]

μ = 100

$\sigma^2 = ¼ * (0^2 + 100^2 + 0^2 + 100^2) = 5000$

Normalized x =

$[0, 100, 0, -100] / \sqrt{5000}$

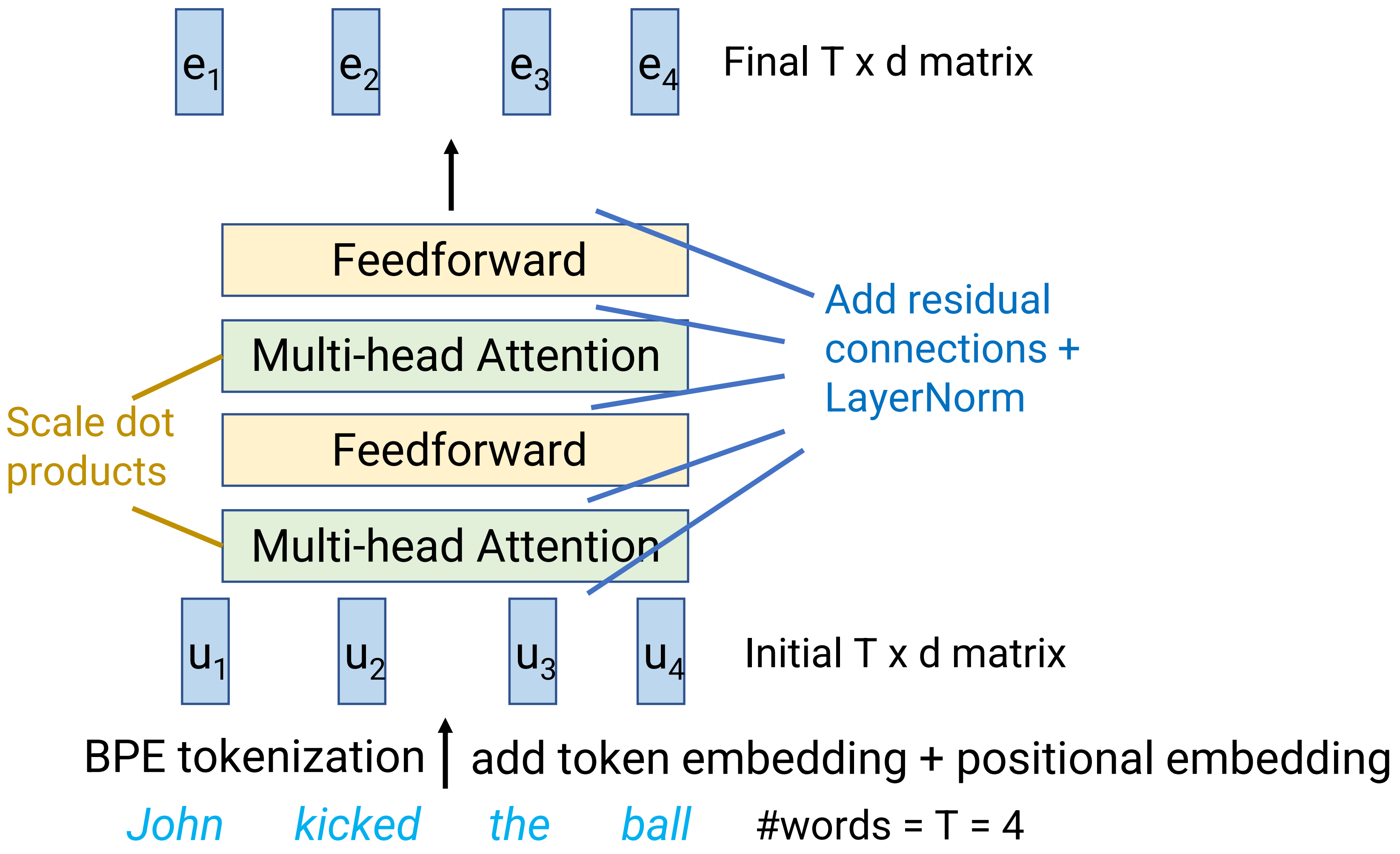
= [0, 1.4, 0, -1.4] (If ε ≈ 0)

Output = [b_1, $1.4a_2+b_2$, b_3, $-1.4a_4+b_4$]

LayerNorm in Transformers

- Add Layer Normalization layer *before* every feedforward & multi-headed attention layer
  - Input: vectors $x_1, \ldots, x_T$
  - Compute μ and σ^2 for each vector
  - Normalize each vector
  - Use the same a and b to scale/shift each vector
  - Output of each layer is $x + \mathrm{Layer}(\mathrm{LayerNorm}(x))$
- Why? Stabilizes optimization by avoiding very large values

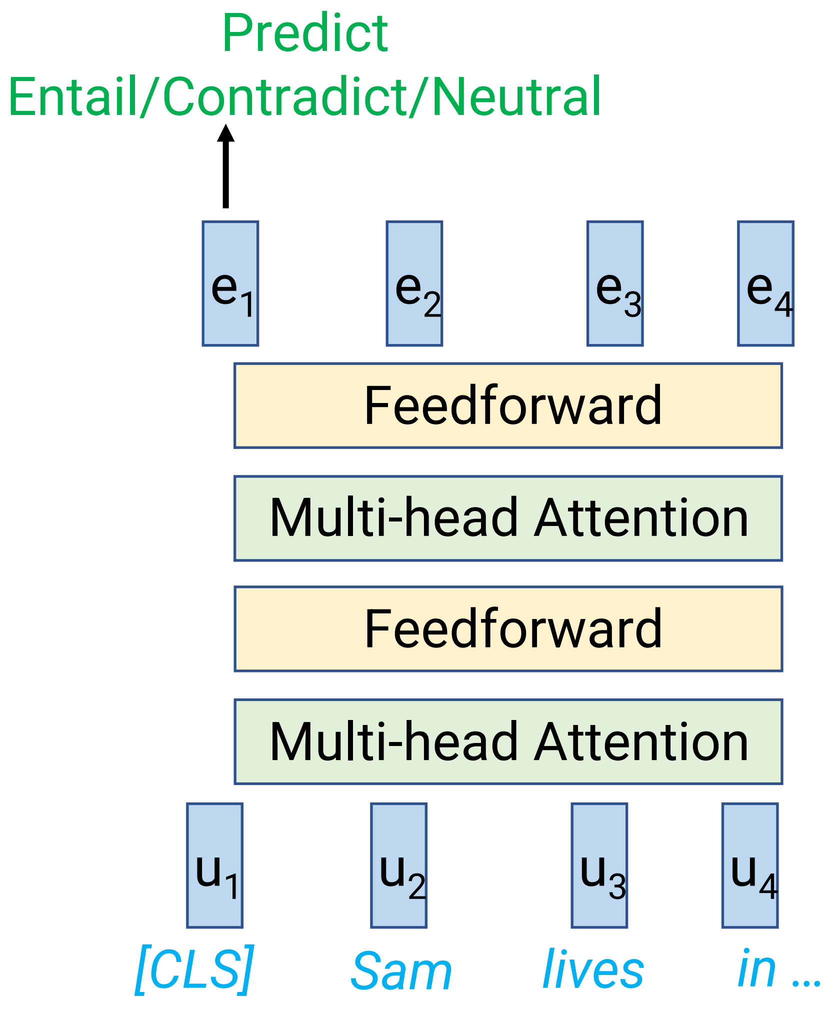
The Full Transformer



Full Transformer also includes bells and whistles:

- Byte pair encoding
- Scaled dot product attention
- Residual connections between layers
- LayerNorm

Training a Transformer



[CLS] Sam lives in Los Angeles. Sam lives in California.

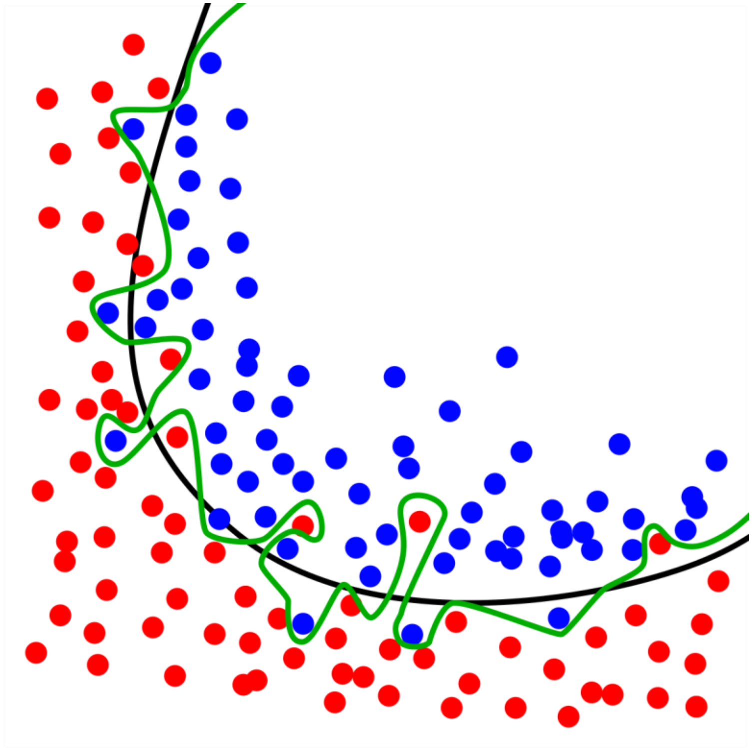
- Example task: Natural Language Inference
  - Input: 2 sentences, A and B
  - Output: 3-way classification: A entails B, A contradicts B, neither
  - Performing this task well requires understanding meaning of sentences + logical relationships
- Input to Transformer: Concatenate special "CLS" token and 2 sentences together
- Output: Use CLS token's final representation to predict
- Train on labeled data, learn to make good predictions

Today's Plan

- Transformers in full detail
- Pre-training
- Transformer decoders
- Vision Transformers

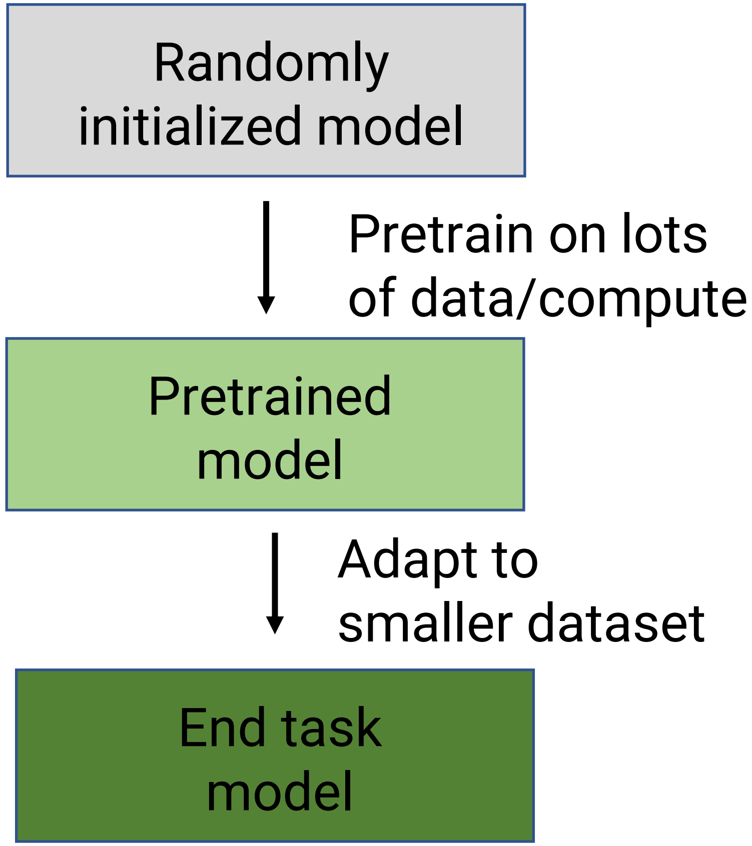
Neural Networks and Scale

- Neural networks are very expressive, but have tons of parameters
  - Very easy to overfit a small training dataset
- Traditionally, neural networks were viewed as flexible but very **“sample-inefficient”**: they need many training examples to be good
  - Computationally expensive
  - Training at scale often uses GPUs

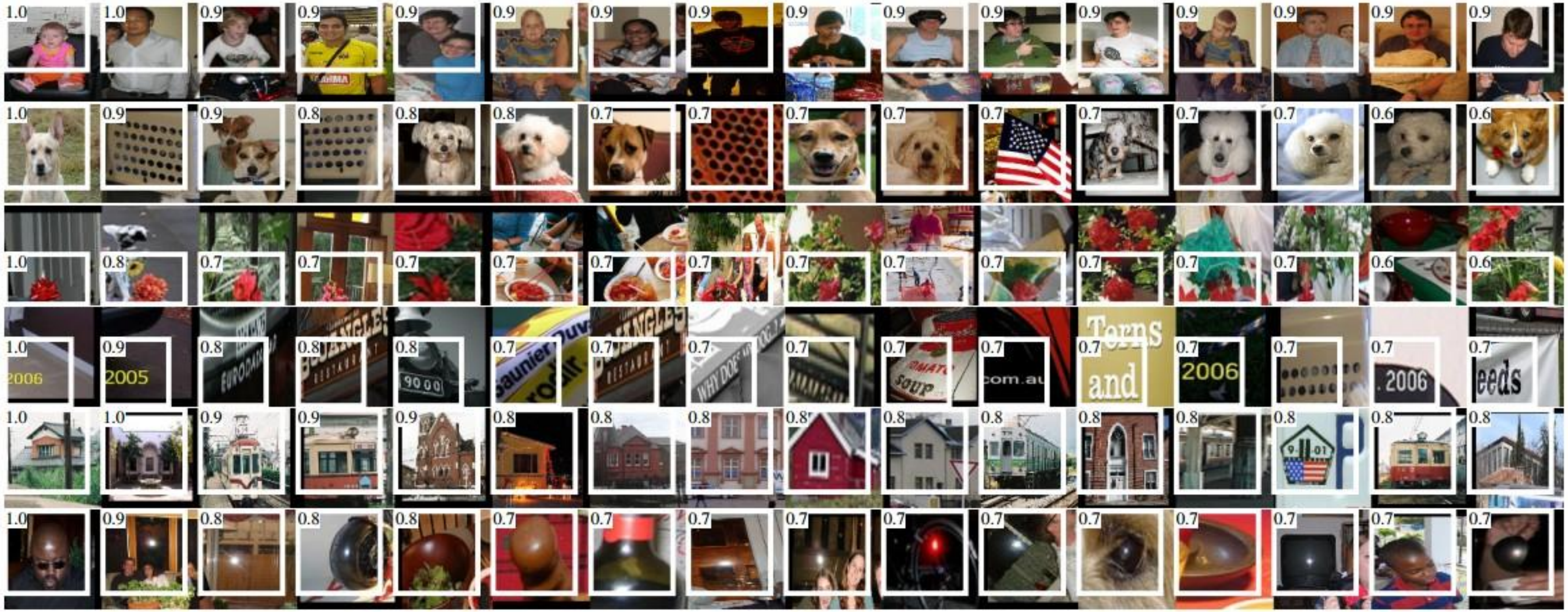


Pretraining

- Neural networks learn to extract features useful for some training task
  - The more data you have, the more successful this will be
- If your training task is very general, these features may also be useful for other tasks!
- Hence: **Pretraining**
  - First pre-train your model on one task with a lot of data
  - Then use model's features for a task with less data
  - Upends the conventional wisdom: You can use neural networks with small datasets now, if they were pretrained appropriately!



ImageNet Features



Faces

Dogs (eyes?)

Red ornaments/
flowers

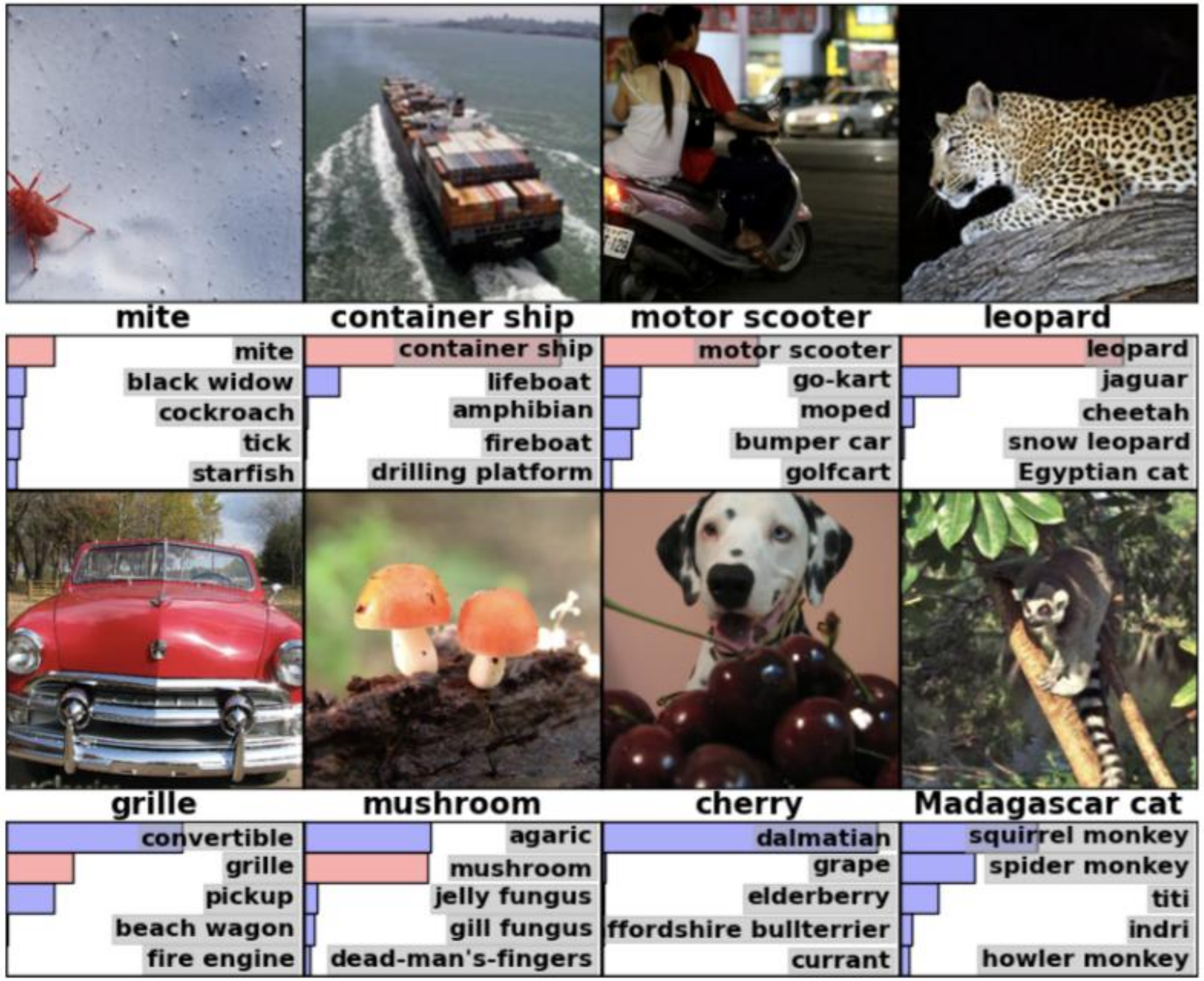
Text (years?)

Houses

Lens flare?

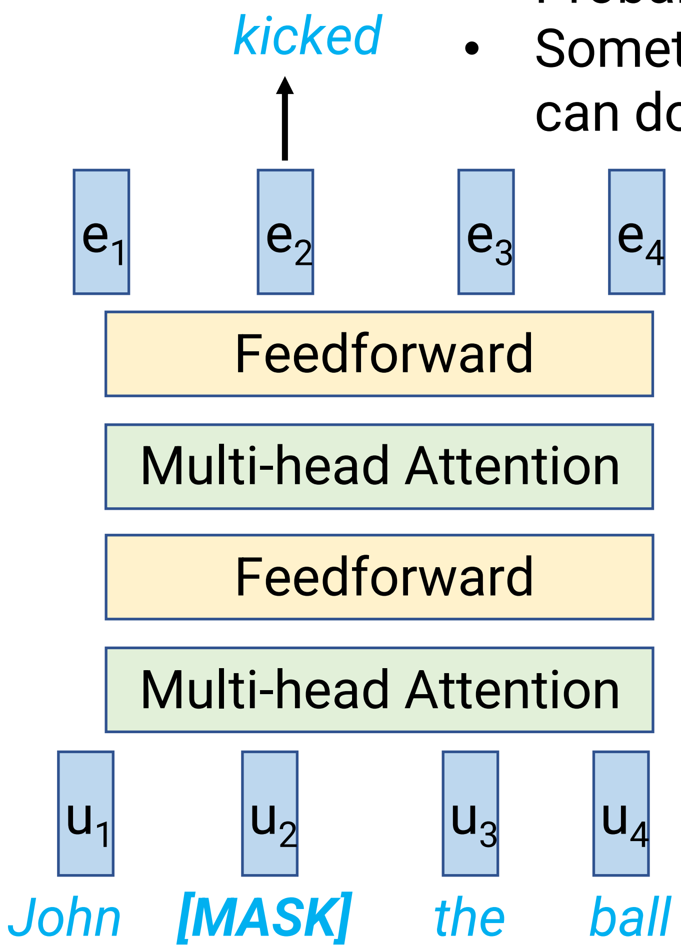
Features learned by AlexNet trained on ImageNet

ImageNet Features



- ImageNet dataset: **14M** images, 1000-way classification
- Most applications don't have this much data
- **But the same features are still useful**
- Using "frozen" pretrained features
  - Get a (small) dataset for your task
  - Generate features from ImageNet-trained model on this data
  - Train linear classifier (or shallow neural network) using ImageNet features

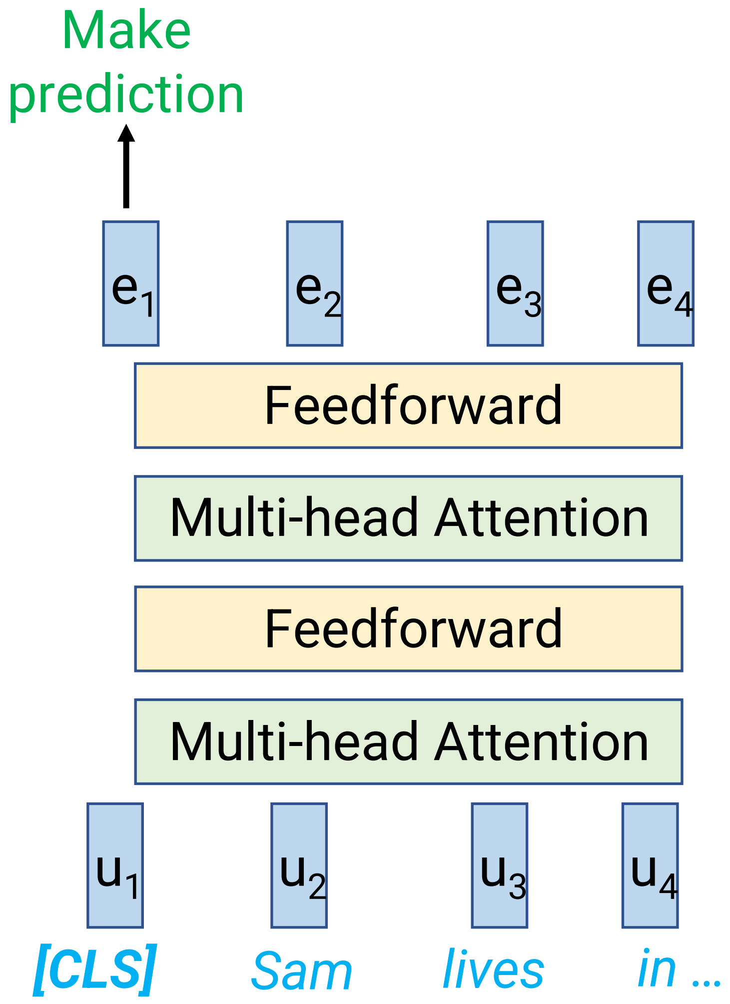
Masked Language Modeling (MLM)



- Probably a verb
- Something a person can do to a ball

- MLM: Randomly mask some words, train model to predict what's missing
  - Doing this well requires understanding grammar, world knowledge, etc.
  - Get training data just by grabbing any text and randomly delete words
  - Thus: Crawl internet for text data
- Transformers are good fit due to scalability
  - Large matrix multiplications are highly optimized on GPUs/TPUs
  - Don't need lots of operations happening in series (like RNNs)
- Most famous example: BERT

Fine-tuning

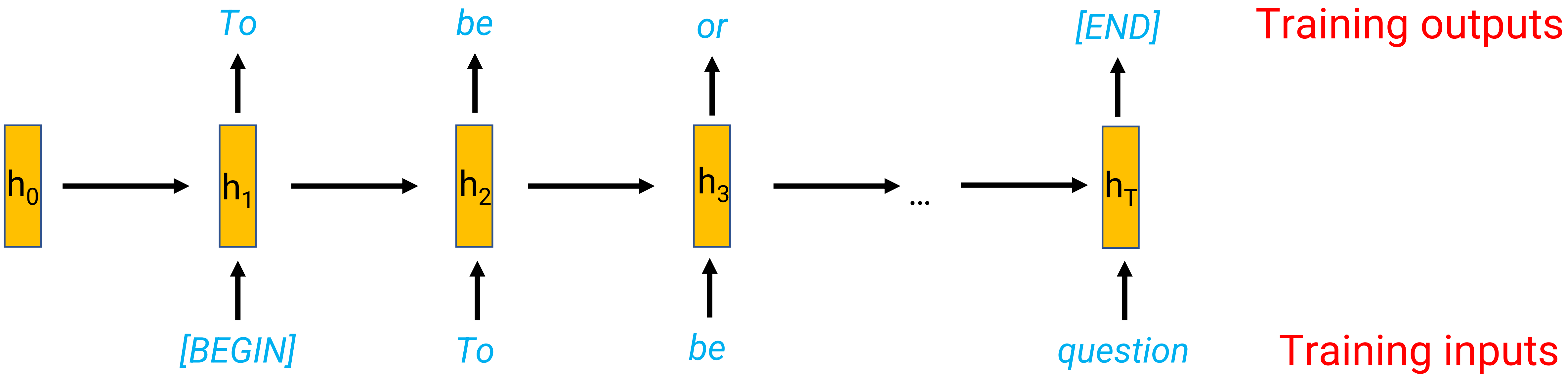


- Initialize parameters with BERT
- Add parameters that take in the output at the [CLS] position and make prediction
- Keep training all parameters (“fine-tune”) on the new task
- Point: BERT provides very good initialization for SGD

Announcements

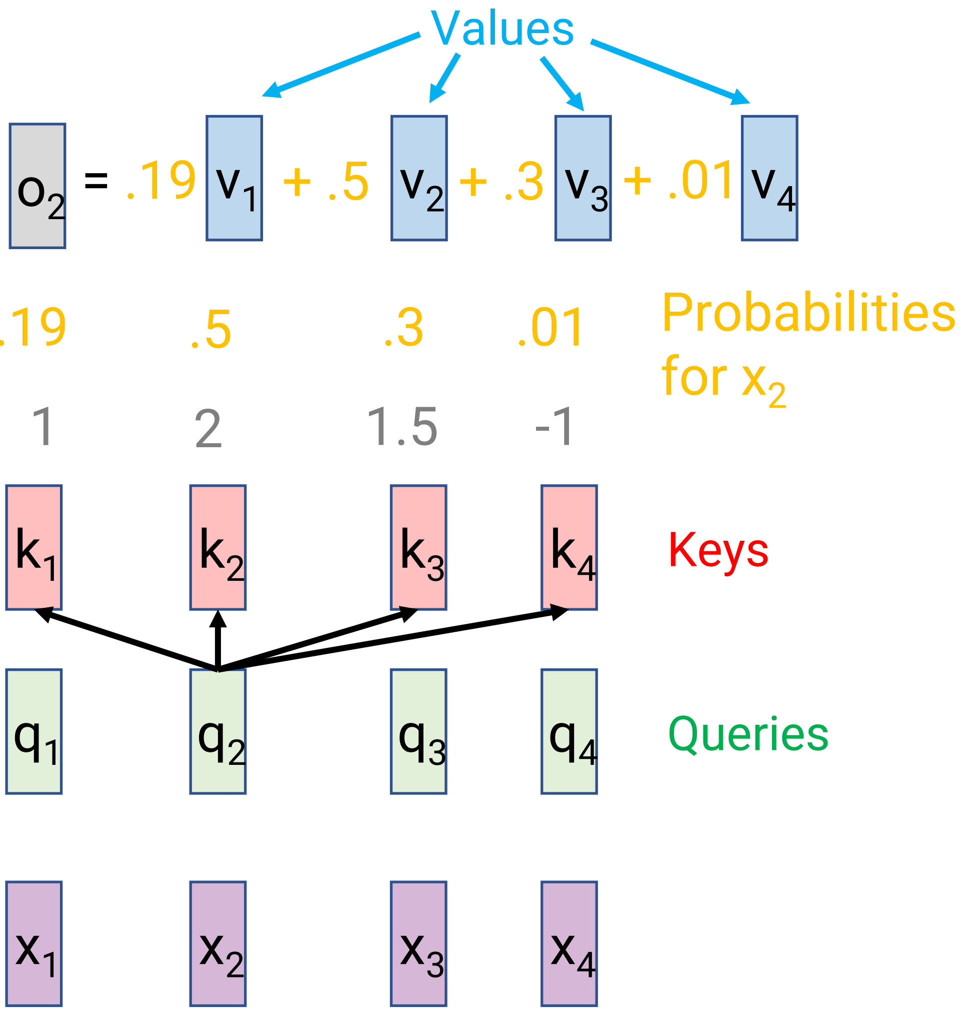
- Project midterm report due Tuesday, April 1
- HW3 released, due Tuesday, April 15
- Tomorrow’s section: RNNs & backpropagation in pytorch
  - How does an RNN decoder work?
  - What do the gradients look like?

Review: RNN Decoder Language Models



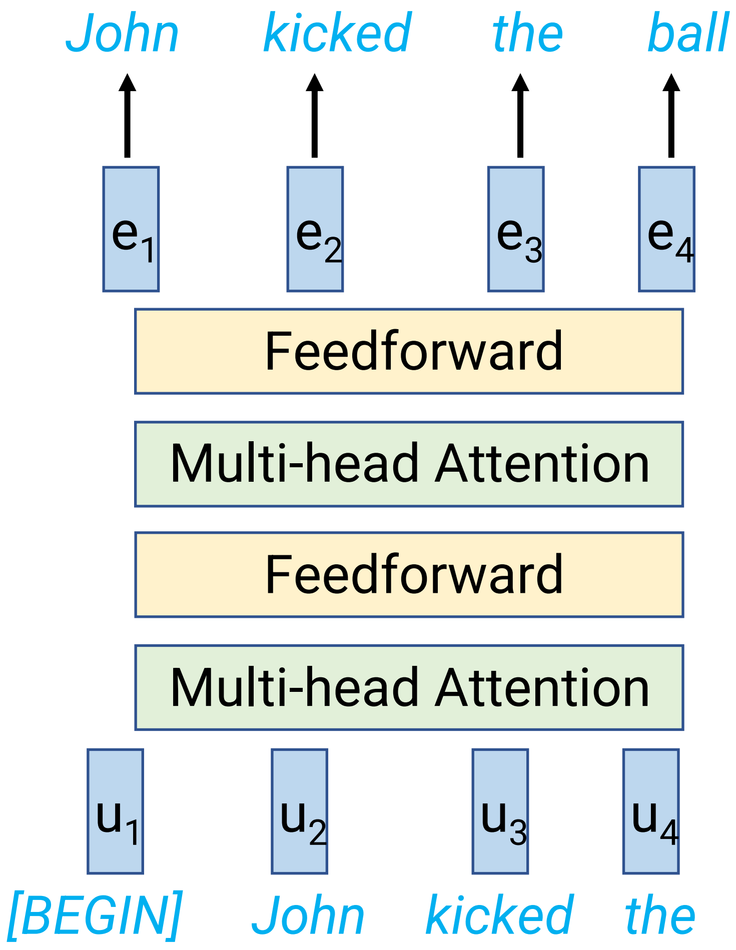
- At each step, predict the next word given current hidden state
- Test time: Model chooses a next word, that gets fed back in
- Training time: Model is fed the human-written words, tries to guess next word at every step
- RNN computations must happen in series at both training and test time
  - Each hidden state depends on the previous hidden state

Transformer autoregressive decoders

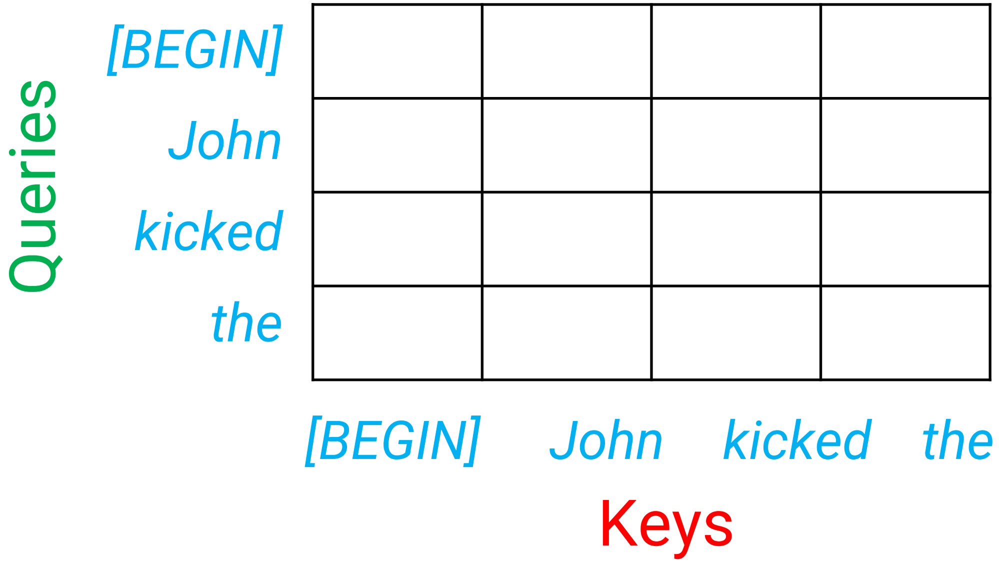


- How can we use Transformers to generate text?
- We will still generate words one at a time
- Problem: The Transformer (encoder) processes all words in parallel
  - Word 2 is allowed to attend to words 3, 4…
  - But in a decoder, words 3, 4, … have not been chosen yet when processing word 2!
- Solution: Use a *variant* of multi-headed attention that **only allows attending to past/current words**
  - Often referred to as “causal masking”: Don’t allow looking into the future

Transformer autoregressive decoders



- Test-time behavior
  - At time t, compute hidden states for current token t by attending to positions 1 through t
  - Each timestep only processes the newest token, attends to previously generated hidden states
  - Happens in series



Transformer autoregressive decoders

- When training a decoder, it has to be "used to" only attending to past/current tokens
- Training time: Masked attention implementation trick
  - Recall: Attention computes Q x K^T (T x T matrix), then does softmax
  - But if generating autoregressively, time t can only attend to times 1 through t
  - Solution: Overwrite Q x K^T to be $-\infty$ when query index < key index
  - **All timesteps happen in parallel**

Queries

[BEGIN]	10	-2	6	3
John	0	7	2	-4
kicked	-3	4	5	-8
the	2	1	7	6
	[BEGIN]	*John*	*kicked*	*the*

Keys

Transformer autoregressive decoders

- When training a decoder, it has to be "used to" only attending to past/current tokens
- Training time: Masked attention implementation trick
  - Recall: Attention computes Q x K^T (T x T matrix), then does softmax
  - But if generating autoregressively, time t can only attend to times 1 through t
  - Solution: Overwrite Q x K^T to be $-\infty$ when query index < key index
  - **All timesteps happen in parallel**

Queries

Queries \ Keys	[BEGIN]	John	kicked	the
[BEGIN]	10	-2	6	3
John	0	7	2	-4
kicked	-3	4	5	-8
the	2	1	7	6

Keys

Transformer autoregressive decoders

- When training a decoder, it has to be “used to” only attending to past/current tokens
- Training time: Masked attention implementation trick
  - Recall: Attention computes Q x K^T (T x T matrix), then does softmax
  - But if generating autoregressively, time t can only attend to times 1 through t
  - Solution: Overwrite Q x K^T to be $-\infty$ when query index < key index
  - **All timesteps happen in parallel**

Queries

	[BEGIN]	John	kicked	the
[BEGIN]	10	$-\infty$	$-\infty$	$-\infty$
John	0	7	$-\infty$	$-\infty$
kicked	-3	4	5	$-\infty$
the	2	1	7	6

Keys

Transformer autoregressive decoders

- When training a decoder, it has to be "used to" only attending to past/current tokens
- Training time: Masked attention implementation trick
  - Recall: Attention computes Q x K^T (T x T matrix), then does softmax
  - But if generating autoregressively, time t can only attend to times 1 through t
  - Solution: Overwrite Q x K^T to be $-\infty$ when query index < key index
  - **All timesteps happen in parallel**

Queries \ Keys	[BEGIN]	John	kicked	the
[BEGIN]	1.0	0	0	0
John	.001	.999	0	0
kicked	.001	.356	.643	0
the	.030	.007	.591	.372

What about ChatGPT???

- ChatGPT appears to be a fine-tuned language model
  - Pretrained on autoregressive language modeling
  - Then fine-tuned with a method called RLHF (reinforcement learning from human feedback)
  - We’ll return to this when we talk about reinforcement learning!

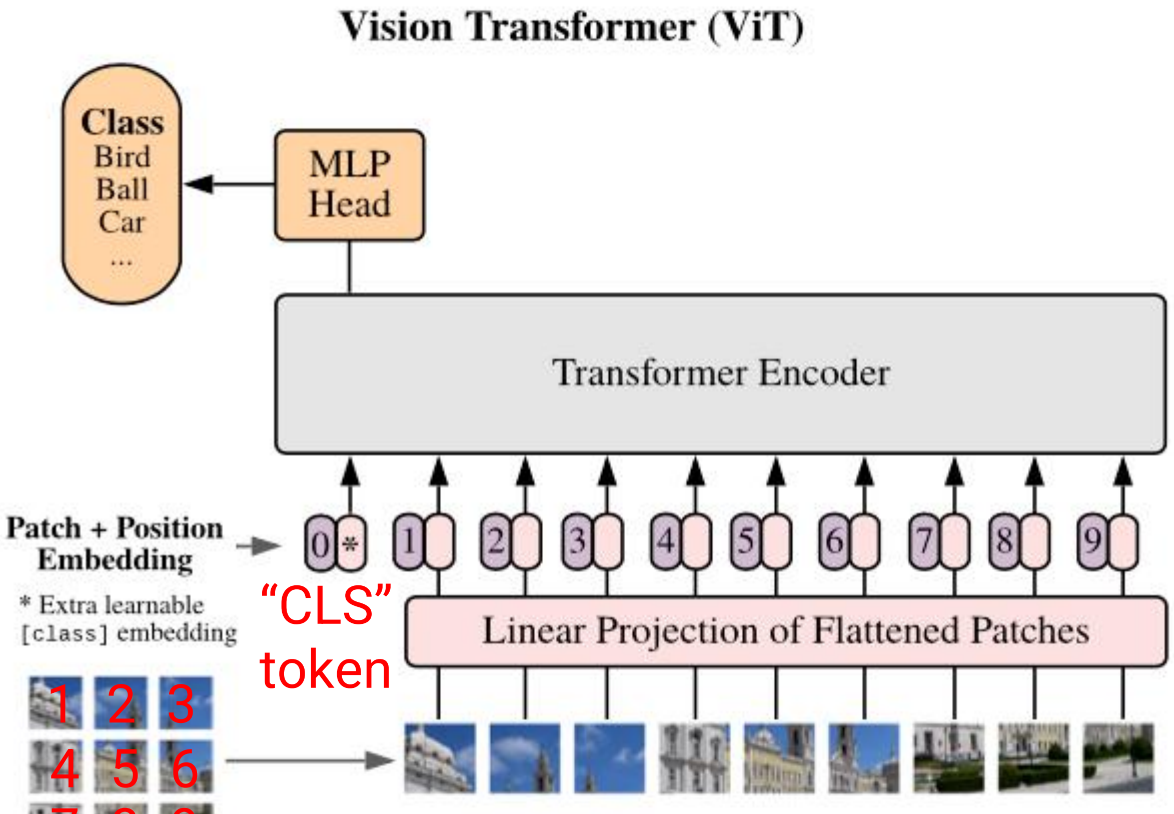
Today's Plan

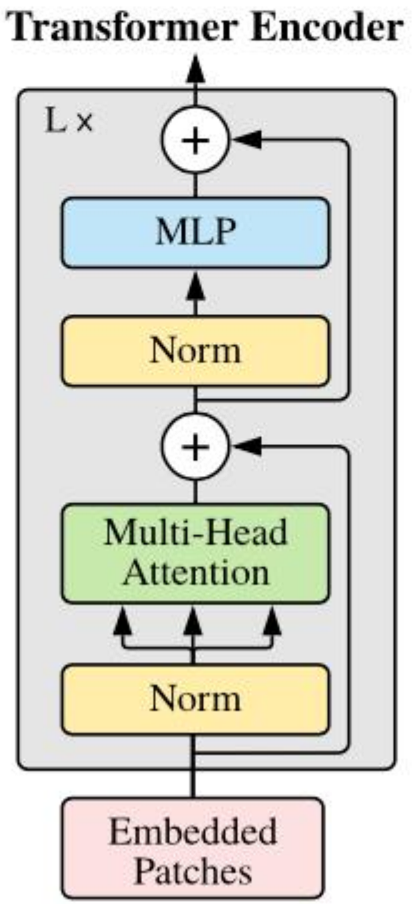
- Transformers in full detail
- Pre-training
- Transformer decoders
- Vision Transformers

Vision Transformers

- Transformers paper came out in 2017
- By 2020, they were widely used in NLP
- Computer vision researchers: What if they’re also good for images?

Vision Transformer





Break image into 16x16 patches

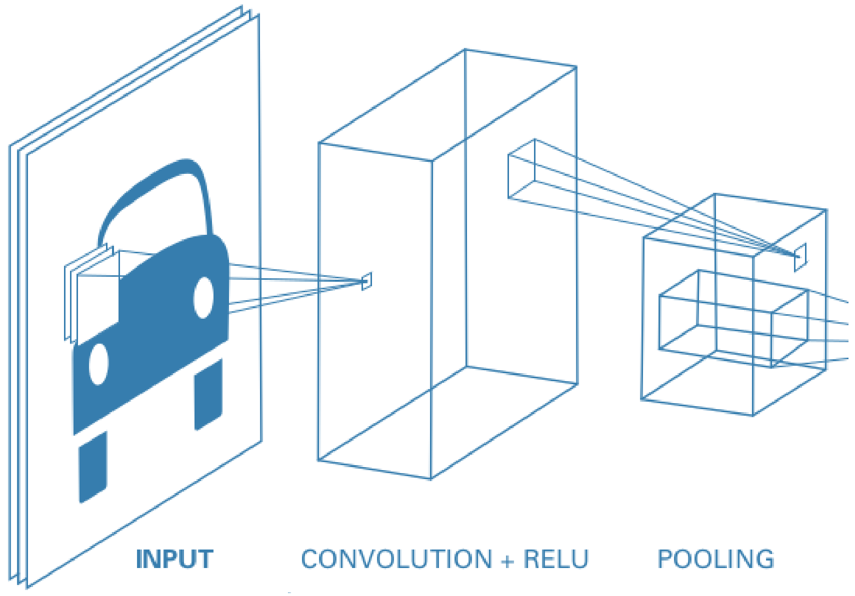
Each patch is a 16x16x3 = 786 dimensional vector; apply a linear layer & add positional embeddings for each patch index

- Break images into square patches ≈ tokens
- Apply a (learned) linear projection to each patch
- Add a "CLS" token
- Add positional embedding for each patch "index"
- Feed to Transformer
- Use final layer CLS representation to make prediction

CNNs vs. Vision Transformers

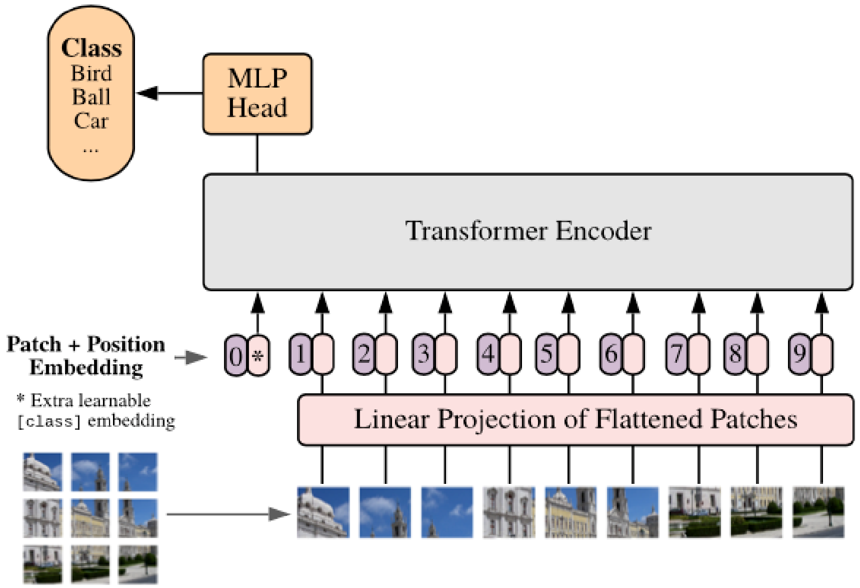
CNN

- Each neuron in 1 layer has a limited receptive field
- Strong "inductive bias": Model has to look locally first, globally later



Vision Transformer

- Each hidden state *can* access information about a faraway part of image via attention
- Weaker "inductive bias"



Conclusion: Transformers

- "Attention is all you need"
  - Get rid of recurrent connections—all "communication" between words in sequence is handled by attention
  - Have multiple attention "heads" to learn different types of relationships between words
    - Each head has its own parameters, which enable them to learn different things
  - Plus lots of additional components to make it fit together
  - Most famous modern language models (e.g., ChatGPT) are Transformers!
- Pretraining
  - First train on large labeled or unlabeled datasets
  - Features learned are useful for other tasks with less data
- Transformers can even be used for images