

A Tutorial on Large Language Models

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MIT

8 weeks

1 hour

Week #	Date	Topic	Lecturer Decision
1	* Thu, Sep 4	Intro + ML refresher	all
2	* Tue, Sep 9	Tokenization & Count-based LMs	Yoon
	* Thu, Sep 11	Count-based LMs (cont.) & Log-Linear Models	Yoon
3	* Tue, Sep 16	Word Representations	Yoon
	* Thu, Sep 18	Neural network / ML basics (FFNs, Optimization, Train/test split, etc.)	Chris
4	* Tue, Sep 23	RNNs	Chris
	* Thu, Sep 25	Attention	Chris
5	* Tue, Sep 30	Transformers	Chris
	* Thu, Oct 2	Advanced Architectures (MoE, Linear RNNs)	Yoon
6	* Tue, Oct 7	Decoding and sampling	Yoon
	* Thu, Oct 9	Midterm review	all
7	* Tue, Oct 14	Midterm	n/a
	* Thu, Oct 16	Beyond next-token prediction (desiderata for modern LMs)	Jacob
8	* Tue, Oct 21	Evaluation	Jacob
	* Thu, Oct 23	Pretraining and SFT	Jacob
9	* Tue, Oct 28	Preference modeling	Jacob
	* Thu, Oct 30	RAG	Jacob
10	* Tue, Nov 4	Chain-of-thought and friends	Chris
	* Thu, Nov 6	LM programming	Omar?
11	* Tue, Nov 11	[Veterans day]	n/a
	* Thu, Nov 13	Efficient training and deployment	Yoon
12	* Tue, Nov 18	Scaling Laws	Yoon
	* Thu, Nov 20	Bias and fairness	Jacob
13	* Tue, Nov 25	Human-in-the-loop and interp	Jacob
	* Thu, Nov 27	[Thanksgiving]	n/a
14	* Tue, Dec 2	Law and policy	Chris Capozzola



Tutorial 10:40–11:40

Yoon Kim
Massachusetts Institute of Techno...
A Tutorial on Large Language Mod...

Part 1: Tokenization

[10 minutes]

Representing text in computers

Byte-pair encoding

Part 2: Language Modeling

[15 minutes]

Formal definition of language modeling

Autoregressive language models

Part 3: Neural Language Models

[20 minutes]

Neural networks for language modeling

Transformers

Part 4: Large Language Models

[15 minutes]

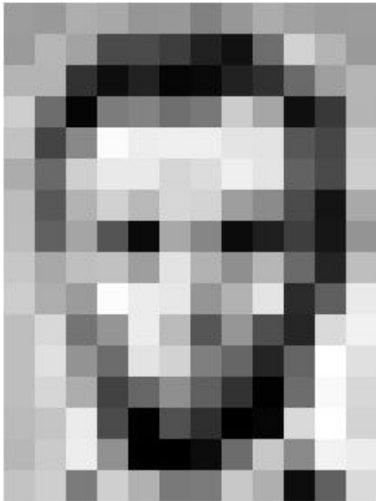
Pre-training & Post-training

LLM-based AI Systems

Part 1: Tokenization

Digital Representations for Computer Vision

How does a computer “see”?



157	153	174	168	150	152	129	151	172	161	155	156
155	182	163	74	75	62	33	17	110	210	180	154
180	180	50	14	34	6	10	33	48	106	159	181
206	109	5	124	131	111	120	204	166	15	56	180
194	68	137	251	237	239	239	228	227	87	71	201
172	105	207	233	233	214	220	239	228	98	74	206
188	88	179	209	185	215	211	158	139	75	20	169
189	97	165	84	10	168	134	11	31	62	22	148
199	168	191	193	158	227	178	143	182	106	36	190
205	174	155	252	236	231	149	178	228	43	95	234
190	216	116	149	236	187	85	150	79	38	218	241
190	224	147	108	227	210	127	102	36	101	255	224
190	214	173	66	103	143	96	96	2	109	249	215
187	196	235	75	1	81	47	0	6	217	255	211
183	202	237	145	0	0	12	108	200	138	243	236
195	206	123	207	177	121	123	200	175	13	96	218

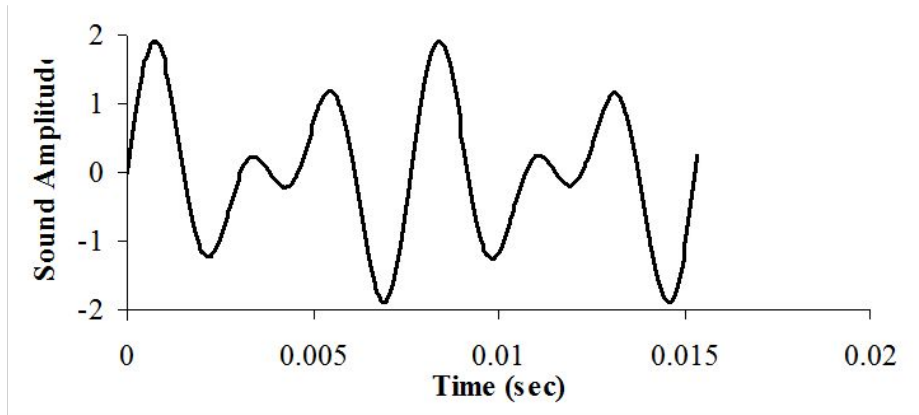
157	153	174	168	150	152	129	151	172	161	155	156
155	182	163	74	75	62	33	17	110	210	180	154
180	180	50	14	34	6	10	33	48	106	159	181
206	109	5	124	131	111	120	204	166	15	56	180
194	68	137	251	237	239	239	228	227	87	71	201
172	105	207	233	233	214	220	239	228	98	74	206
188	88	179	209	185	215	211	158	139	75	20	169
189	97	165	84	10	168	134	11	31	62	22	148
199	168	191	193	158	227	178	143	182	106	36	190
205	174	155	252	236	231	149	178	228	43	95	234
190	216	116	149	236	187	85	150	79	38	218	241
190	224	147	108	227	210	127	102	36	101	255	224
190	214	173	66	103	143	96	96	2	109	249	215
187	196	235	75	1	81	47	0	6	217	255	211
183	202	237	145	0	0	12	108	200	138	243	236
195	206	123	207	177	121	123	200	175	13	96	218

Matrix of integers:
each number
represents pixel
intensity.

$\in \{0, 255\}^{\text{height} \times \text{width}}$

Digital Representations for Audio Processing

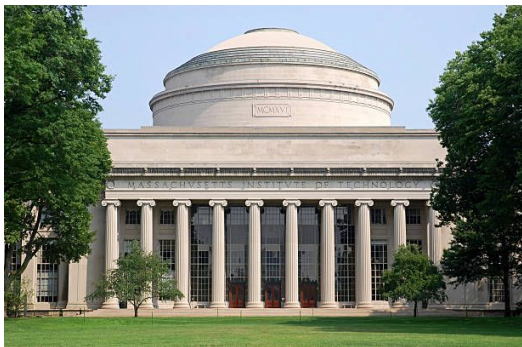
How does a computer “hear”?



$\in \mathbb{R}$

1D vector of numbers, each of which represents the amplitude of air pressure variation at a time point.

Digital Representations for Vision/Audio



$$\in \{0, 255\}^{h \times w \times 3}$$

Images and audio admit “native” digital representations where the values “mean” something.



$$\in \mathbb{R}$$

Digital Representations for Natural Language Processing?

How do we represent strings?

Hello world!

Digital Representations for Natural Language Processing

How do we represent strings?

Hello world!

A lookup table that maps characters
to integers

Character	Integer (8 bits)
a	97
b	98
c	99
⋮	⋮
⌊	32
!	33
⋮	⋮

Digital Representations for Natural Language Processing

How do we represent strings?

Hello world!

A lookup table that maps characters to integers

Character	Integer (8 bits)
a	97
b	98
c	99
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␣	32
!	33
⋮	⋮

Character:	H	e	l	l	o	␣	w	o	r	l	d	!
Integer:	72	101	108	108	111	32	119	111	114	108	100	33

Digital Representations for Natural Language Processing

How do we represent strings?

Hello world!

A lookup table that maps characters to integers

ASCII: 128 values
UTF-8: 256 values

Character	Integer (8 bits)
a	97
b	98
c	99
⋮	⋮
⌊	32
!	33
⋮	⋮

Character:	H	e	l	l	o	⌊	w	o	r	l	d	!
Integer:	72	101	108	108	111	32	119	111	114	108	100	33

Potential Issues

Unlike in images/audio, encoding is arbitrary.

Character	Integer (8 bits)
a	97
b	98
c	99
⋮	⋮
⌋	32
!	33
⋮	⋮

Fundamental issue when working with domains such as language where there is (mostly) no connection between form and meaning (*linguistic arbitrariness*).

Potential Issues

More practical issue: such “raw” encodings lead to large input sizes

The government shutdown was delayed indefinitely

Input length = 48 (if working with characters)

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More practical issue: such “raw” encodings lead to large input sizes

The government shutdown was delayed indefinitely

Input length = 48 (if working with characters)

The training/deployment cost of deep learning models often depends on input length

→ character-level models are *inefficient*.

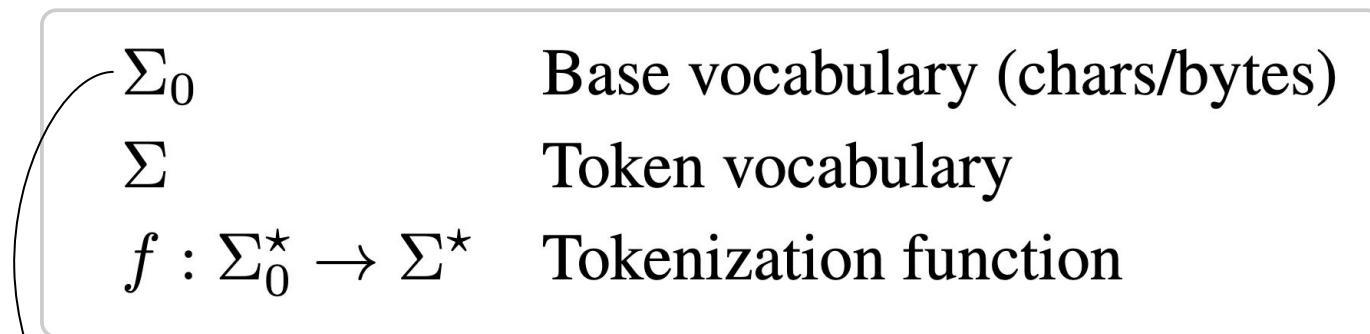
Tokenization

The process of converting raw bytes into larger units called **tokens**.

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Involves selecting/learning a **token vocabulary** along with a **tokenization function**.



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Tokenization

The process of converting raw bytes into larger units called **tokens**.

Involves selecting/learning a **token vocabulary** along with a **tokenization function**.

Σ_0	Base vocabulary (chars/bytes)
Σ	Token vocabulary
$f : \Sigma_0^* \rightarrow \Sigma^*$	Tokenization function

The first step when working with any text data (including for building LLMs).

Word-level Tokenization

The government shutdown was delayed indefinitely



[The, `▯`government, `▯`shutdown, `▯`was, `▯`delayed, `▯`indefinitely]

[7, 1266, 3435, 853, 444, 49766]

- ✓ Simple
- ✓ “Makes sense” linguistically (words *exist*)

Word-level Tokenization

Tokenization Scheme	Vocabulary Σ	Length of Encoding $ f(\text{Hello world!}) $
Chars (bytes)	$\Sigma = \{\sqcup, a, b, \dots\}$ $ \Sigma = 256$	12
Words	$\Sigma = \{a, \text{aardvark}, \dots, \text{zyzzyva}, !, .\}$ $ \Sigma \approx 50000$	3

Word-level Tokenization: Issues

Word-level vocabulary is not really finite.

There are `131392814871` reasons to take NLP.

He's `vibecoding` to build his new AI start-up.

`Massachusetts` Institute of Technology is in `Cambridge`.

Word-level Tokenization: Issues

Word-level vocabulary is not really finite.

There are `131392814871` reasons to take NLP.

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Many languages don't use white space to tokenize.

我喜欢吃苹果

昨日友達と映画を見に行きました

“Optimal” Tokenization?

Suppose you are given training set \mathbf{X} and a desired vocab size $|\Sigma|$.

```
['I', ' ', 's', 'e', 'e', ' ', 'a', ' ', 'b', 'e', 'a', 'u', 't', 'i', 'f', 'u', 'l', ' ',  
'c', 'i', 't', 'y', ' ', 'a', 'n', 'd', ' ', 'a', ' ', 'b', 'r', 'i', 'l', 'l', 'i', 'a',  
'n', 't', ' ', 'p', 'e', 'o', 'p', 'l', 'e', ' ', 'r', 'i', 's', 'i', 'n', 'g', ' ', 'f',  
'r', 'o', 'm', ' ', 't', 'h', 'i', 's', ' ', 'a', 'b', 'y', 's', 's', ' ', ' ', 'a', 'n',  
'd', ' ', ' ', ' ', 'i', 'n', ' ', 't', 'h', 'e', 'i', 'r', ' ', 's', 't', 'r', 'u', 'g', 'g',  
'l', 'e', 's', ' ', 't', 'o', ' ', 'b', 'e', ' ', 't', 'r', 'u', 'l', 'y', ' ', 'f', 'r',  
'e', 'e', ' ', ' ', 'i', 'n', ' ', 't', 'h', 'e', 'i', 'r', ' ', 't', 'r', 'i', 'u', 'm',  
'p', 'h', 's', ' ', 'a', 'n', 'd', ' ', 'd', 'e', 'f', 'e', 'a', 't', 's', ' ', ' ', 't',  
'h', 'r', 'o', 'u', 'g', 'h']
```

```
[73, 32, 115, 101, 101, 32, 97, 32, 98, 101, 97, 117, 116, 105, 102, 117, 108, 32, 99, 105,  
116, 121, 32, 97, 110, 100, 32, 97, 32, 98, 114, 105, 108, 108, 105, 97, 110, 116, 32, 112,  
101, 111, 112, 108, 101, 32, 114, 105, 115, 105, 110, 103, 32, 102, 114, 111, 109, 32, 116,  
104, 105, 115, 32, 97, 98, 121, 115, 115, 44, 32, 97, 110, 100, 44, 32, 105, 110, 32, 116,  
104, 101, 105, 114, 32, 115, 116, 114, 117, 103, 103, 108, 101, 115, 32, 116, 111, 32, 98,  
101, 32, 116, 114, 117, 108, 121, 32, 102, 114, 101, 101, 44, 32, 105, 110, 32, 116, 104,  
101, 105, 114, 32, 116, 114, 105, 117, 109, 112, 104, 115, 32, 97, 110, 100, 32, 100, 101,  
102, 101, 97, 116, 115, 44, 32, 116, 104, 114, 111, 117, 103, 104]
```

What is an “optimal” tokenization function?

“Optimal” Tokenization?

What is an “optimal” tokenization function?

Σ_0	Base vocabulary (chars/bytes)
Σ	Token vocabulary
$f : \Sigma_0^* \rightarrow \Sigma^*$	Tokenization function

$$\min_{\Sigma, f} |f(\mathbf{X})|$$

$$\text{such that } |\Sigma| = V$$

Byte Pair Encoding: An Approximation

Byte-Pair Encoding: Use a learned vocabulary of **subwords** as the fundamental unit → Can deal with unseen words, but not as inefficient as characters.

Byte Pair Encoding: An Approximation

Byte-Pair Encoding: Use a learned vocabulary of **subwords** as the fundamental unit → Can deal with unseen words, but not as inefficient as characters.

Input: Text corpus **X**, desired vocabulary size **N**

Algorithm:

While vocabulary size < N:

 Find most frequent pair of tokens in **X**

 (**a**, **b**)

 Make a new entry in dictionary

new_tok = **ab**

 Replace all occurrences

ab replaced with **new_tok**

Byte Pair Encoding: Example

The feral cat attacked my cat. My cat bit the attacking cat.

```
['T', 'h', 'e', ' ', 'f', 'e', 'r', 'a', 'l', ' ', 'c', 'a', 't', ' ', 'a', 't', 't', 'a', 'c', 'k',  
'e', 'd', ' ', 'm', 'y', ' ', 'c', 'a', 't', '.', ' ', 'M', 'y', ' ', 'c', 'a', 't', ' ', 'b', 'i',  
't', ' ', 't', 'h', 'e', ' ', 'a', 't', 't', 'a', 'c', 'k', 'i', 'n', 'g', ' ', 'c', 'a', 't', '.']
```

Byte Pair Encoding: Example

The feral **cat** attacked my **cat**. My **cat** bit the **attacking cat**.

Merged pair ['T', 'h', 'e', ' ', 'f', 'e', 'r', 'a', 'l', ' ', 'c', 'a', 't', ' ', 'a', 't', 't', 'a', 'c', 'k',
'e', 'd', ' ', 'm', 'y', ' ', 'c', 'a', 't', '.', ' ', 'M', 'y', ' ', 'c', 'a', 't', ' ', 'b', 'i',
't', ' ', 't', 'h', 'e', ' ', 'a', 't', 't', 'a', 'c', 'k', 'i', 'n', 'g', ' ', 'c', 'a', 't', '.']
'at'

Byte Pair Encoding: Example

The feral cat attacked my cat. My cat bit the attacking cat.

Merged pair

```
['T', 'h', 'e', ' ', 'f', 'e', 'r', 'a', 'l', ' ', 'c', 'a', 't', ' ', 'a', 't', 't', 'a', 'c', 'k',  
'e', 'd', ' ', 'm', 'y', ' ', 'c', 'a', 't', '.', ' ', 'M', 'y', ' ', 'c', 'a', 't', ' ', 'b', 'i',  
't', ' ', 't', 'h', 'e', ' ', 'a', 't', 't', 'a', 'c', 'k', 'i', 'n', 'g', ' ', 'c', 'a', 't', '.']
```

'at'

```
['T', 'h', 'e', ' ', 'f', 'e', 'r', 'a', 'l', ' ', 'c', 'at', ' ', 'at', 't', 'a', 'c', 'k', 'e',  
'd', ' ', 'm', 'y', ' ', 'c', 'at', '.', ' ', 'M', 'y', ' ', 'c', 'at', ' ', 'b', 'i', 't', ' ', 't',  
'h', 'e', ' ', 'at', 't', 'a', 'c', 'k', 'i', 'n', 'g', ' ', 'c', 'at', '.']
```

Byte Pair Encoding: Example

The feral cat attacked my cat. My cat bit the attacking cat.

Merged pair

```
['T', 'h', 'e', ' ', 'f', 'e', 'r', 'a', 'l', ' ', 'c', 'a', 't', ' ', 'a', 't', 't', 'a', 'c', 'k',  
'e', 'd', ' ', 'm', 'y', ' ', 'c', 'a', 't', '.', ' ', 'M', 'y', ' ', 'c', 'a', 't', ' ', 'b', 'i',  
't', ' ', 't', 'h', 'e', ' ', 'a', 't', 't', 'a', 'c', 'k', 'i', 'n', 'g', ' ', 'c', 'a', 't', '.']
```

'at'

```
['T', 'h', 'e', ' ', 'f', 'e', 'r', 'a', 'l', ' ', 'c', 'at', ' ', 'at', 't', 'a', 'c', 'k', 'e',  
'd', ' ', 'm', 'y', ' ', 'c', 'at', '.', ' ', 'M', 'y', ' ', 'c', 'at', ' ', 'b', 'i', 't', ' ', 't',  
'h', 'e', ' ', 'at', 't', 'a', 'c', 'k', 'i', 'n', 'g', ' ', 'c', 'at', '.']
```

' c'

```
['T', 'h', 'e', ' ', 'f', 'e', 'r', 'a', 'l', ' c', 'at', ' ', 'at', 't', 'a', 'c', 'k', 'e', 'd', ' ',  
' ', 'm', 'y', ' c', 'at', '.', ' ', 'M', 'y', ' c', 'at', ' ', 'b', 'i', 't', ' ', 't', 'h', 'e', ' ',  
'at', 't', 'a', 'c', 'k', 'i', 'n', 'g', ' c', 'at', '.']
```

Byte Pair Encoding: Example

The feral cat attacked my cat. My cat bit the attacking cat.

Merged pair

```
['T', 'h', 'e', ' ', 'f', 'e', 'r', 'a', 'l', ' ', 'c', 'a', 't', ' ', 'a', 't', 't', 'a', 'c', 'k',  
'e', 'd', ' ', 'm', 'y', ' ', 'c', 'a', 't', '.', ' ', 'M', 'y', ' ', 'c', 'a', 't', ' ', 'b', 'i',  
't', ' ', 't', 'h', 'e', ' ', 'a', 't', 't', 'a', 'c', 'k', 'i', 'n', 'g', ' ', 'c', 'a', 't', '.']
```

'at'

```
['T', 'h', 'e', ' ', 'f', 'e', 'r', 'a', 'l', ' ', 'c', 'at', ' ', 'at', 't', 'a', 'c', 'k', 'e',  
'd', ' ', 'm', 'y', ' ', 'c', 'at', '.', ' ', 'M', 'y', ' ', 'c', 'at', ' ', 'b', 'i', 't', ' ', 't',  
'h', 'e', ' ', 'at', 't', 'a', 'c', 'k', 'i', 'n', 'g', ' ', 'c', 'at', '.']
```

' c'

```
['T', 'h', 'e', ' ', 'f', 'e', 'r', 'a', 'l', ' c', 'at', ' ', 'at', 't', 'a', 'c', 'k', 'e', 'd', ' ',  
' ', 'm', 'y', ' c', 'at', '.', ' ', 'M', 'y', ' c', 'at', ' ', 'b', 'i', 't', ' ', 't', 'h', 'e', ' ',  
'at', 't', 'a', 'c', 'k', 'i', 'n', 'g', ' c', 'at', '.']
```

' cat'

```
['T', 'h', 'e', ' ', 'f', 'e', 'r', 'a', 'l', ' cat', ' ', 'at', 't', 'a', 'c', 'k', 'e', 'd', ' ',  
'm', 'y', ' cat', '.', ' ', 'M', 'y', ' cat', ' ', 'b', 'i', 't', ' ', 't', 'h', 'e', ' ', 'at', 't',  
'a', 'c', 'k', 'i', 'n', 'g', ' cat', '.']
```

Byte Pair Encoding: Example

The feral cat attacked my cat. My cat bit the attacking cat.

```
['T', 'h', 'e', ' ', 'f', 'e', 'r', 'a', 'l', ' ', 'c', 'a', 't', ' ', 'a', 't', 't', 'a', 'c', 'k',  
'e', 'd', ' ', 'm', 'y', ' ', 'c', 'a', 't', '.', ' ', 'M', 'y', ' ', 'c', 'a', 't', ' ', 'b', 'i',  
't', ' ', 't', 'h', 'e', ' ', 'a', 't', 't', 'a', 'c', 'k', 'i', 'n', 'g', ' ', 'c', 'a', 't','.']
```

**After 11
merges**

```
['T', 'he ', 'f', 'e', 'r', 'a', 'l', ' cat ', 'attack', 'e', 'd', ' ', 'm', 'y', ' cat.', ' ', 'M',  
'y', ' cat ', 'b', 'i', 't', ' ', 't', 'he ', 'attack', 'i', 'n', 'g', ' cat.']
```

Length reduction: 60 → 30.

Byte Pair Encoding: Example

The feral cat attacked my cat. My cat bit the attacking cat.

```
['T', 'h', 'e', ' ', 'f', 'e', 'r', 'a', 'l', ' ', 'c', 'a', 't', ' ', ' ', 'a', 't', 't', 'a', 'c', 'k',  
'e', 'd', ' ', ' ', 'm', 'y', ' ', ' ', 'c', 'a', 't', '.', ' ', ' ', 'M', 'y', ' ', ' ', 'c', 'a', 't', ' ', ' ', 'b', 'i',  
't', ' ', ' ', 't', 'h', 'e', ' ', ' ', 'a', 't', 't', 'a', 'c', 'k', 'i', 'n', 'g', ' ', ' ', 'c', 'a', 't', '.']
```

After 11
merges

```
['T', 'he ', 'f', 'e', 'r', 'a', 'l', ' cat ', 'attack', 'e', 'd', ' ', ' ', 'm', 'y', ' cat.', ' ', ' ', 'M',  
'y', ' cat ', 'b', 'i', 't', ' ', ' ', 't', 'he ', 'attack', 'i', 'n', 'g', ' cat.']
```

Length reduction: 60 → 30.

BPE vocabulary Σ

```
{  
  '\x00', '\x01', ..., ' ', '!', '"', '#', '$', '%', '&', "'", '(', ')', '*', '+', ',',  
  '-', '.', '/', '0', '1', '2', '3', '4', '5', '6', '7', '8', '9', ':', ';', '<', '=',  
'>', '?', '@', 'A', 'B', 'C', 'D', 'E', 'F', 'G', 'H', 'I', 'J', 'K', 'L', 'M', 'N',  
'O', 'P', 'Q', 'R', 'S', 'T', 'U', 'V', 'W', 'X', 'Y', 'Z', '[', '\\', ']', '^', '_',  
'`', 'a', 'b', 'c', 'd', 'e', 'f', 'g', 'h', 'i', 'j', 'k', 'l', 'm', 'n', 'o', 'p',  
'q', 'r', 's', 't', 'u', 'v', 'w', 'x', 'y', 'z', '{', '|', '}', '~', '\x7f',  
  'at', ' c', ' cat', 'he', 'he ', ' cat ', 'att', 'atta', 'attac', 'attack', ' cat.'  
}
```

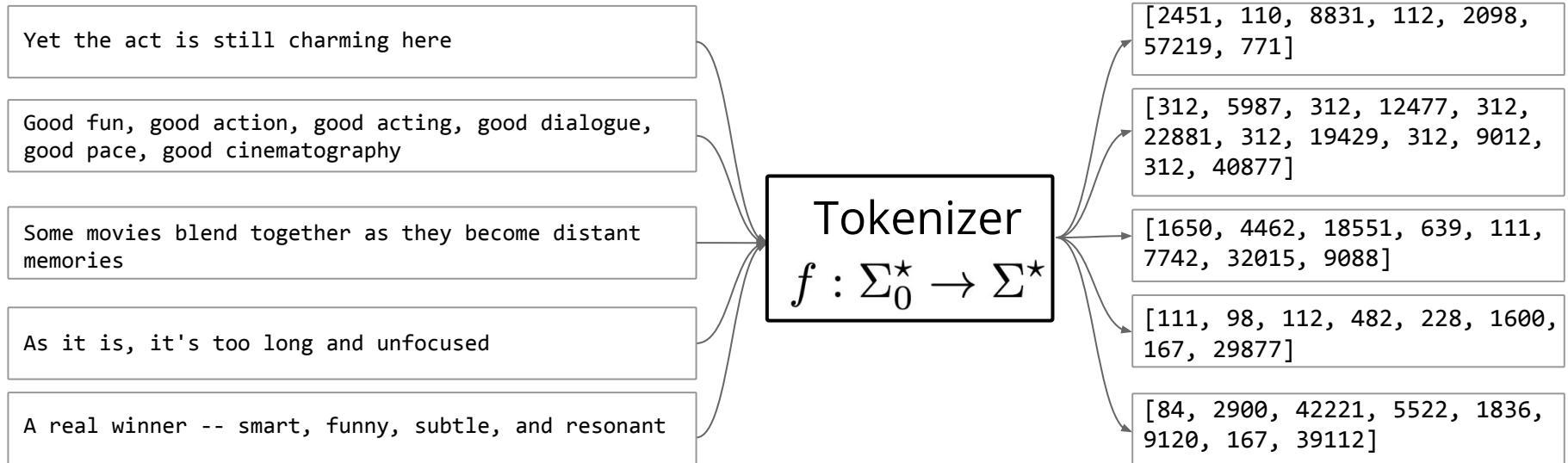
Original
character
vocabulary Σ_0

New tokens

Byte Pair Encoding

Tokenization is the first step in building LLMs:

- Apply BPE on large text dataset to get a subword vocabulary (32K–128K)
- Tokenize the dataset to convert text into integers.



Part 1 Takeaway

Tokenization converts text into sequences of integers.

Raw characters are too inefficient to work with. Words are too “high level”.

Byte-pair encoding offers a middle ground: can still encode words as a single unit (if they occur often enough), but also represent unknown words.

Learning a BPE vocabulary and using it to convert text into integers is the first step in building LLMs (and NLP more broadly).

Part 2: Language Modeling

Language Model

Language Model: a probability distribution over strings in a language.

$$p(x)$$

$$x = x_1 x_2 \dots x_T$$

Language Model

Language Model: a probability distribution over strings in a language.

$$p(\text{I'm not a cat}) = 0.00000004$$

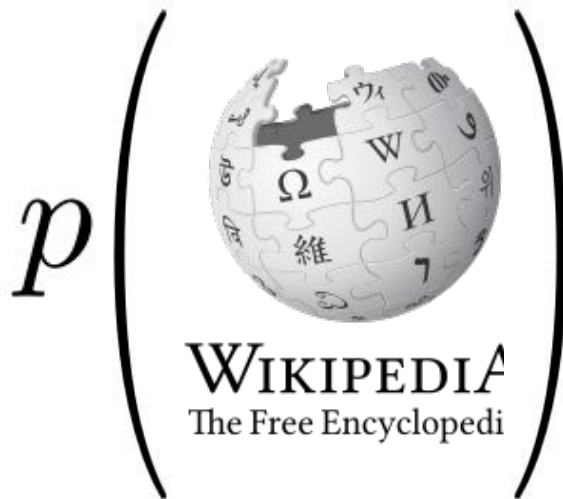
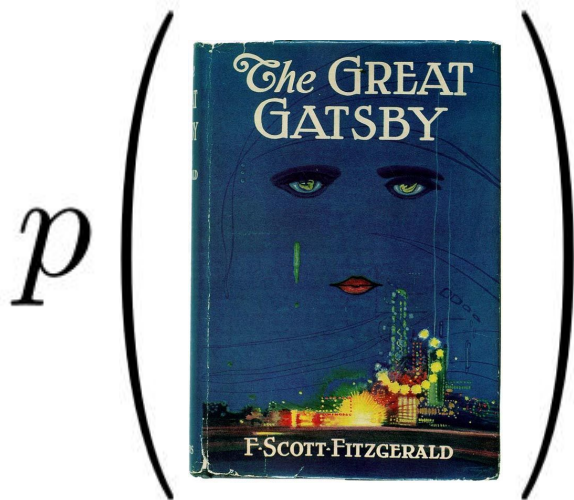


$$p(\text{He is hungry}) = 0.000025$$

$$p(\text{Dog the asd@sdf 1124 !?}) \approx 0$$

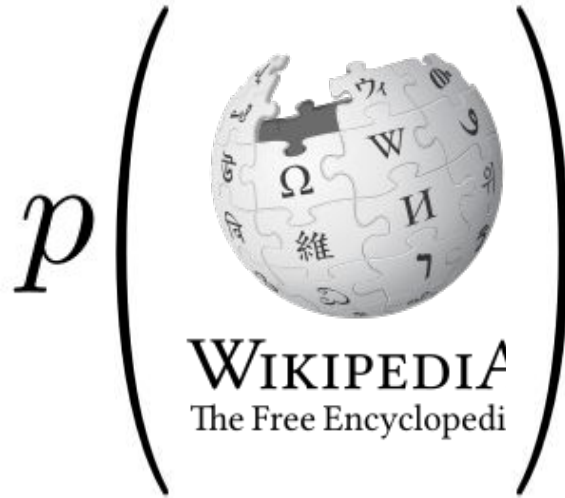
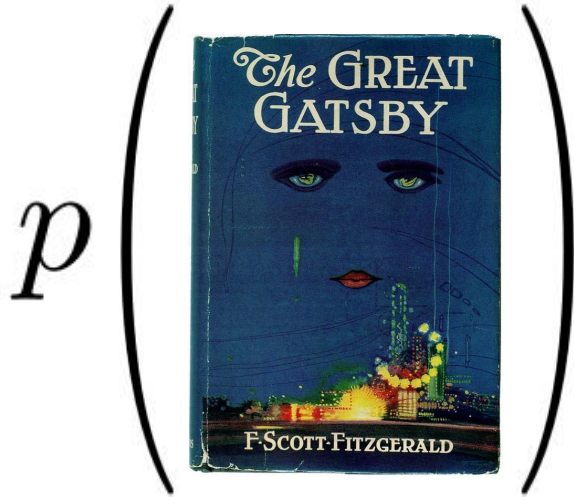
Language Model

Language Model: a probability distribution over strings in a language.



Language Model

Language Model: a probability distribution over ~~strings in a language~~
sequences of tokens integers



Language Modeling

Language Modeling: the task of estimating this distribution from data

Language Modeling

Language Modeling: the task of estimating this distribution from data

- Define a statistical model $p_{\theta}(x)$ with parameters θ
- Given a training set $x = x_1x_2 \dots x_T$

$$\arg \max_{\theta} p_{\theta}(x_1x_2 \dots x_T)$$

(Can view the training set a very long sequence of tokens, or a set of sequences.)

Language Modeling

Language Modeling: the task of estimating this distribution from data

- Define a statistical model $p_{\theta}(x)$ with parameters θ
- Given a training set $x = x_1x_2 \dots x_T$

$$\arg \max_{\theta} p_{\theta}(x_1x_2 \dots x_T)$$

(Can view the training set a very long sequence of tokens, or a set of sequences.)

Simple maximum likelihood learning!

Language Model Factorization

Need to **decompose** (factorize) this joint distribution.

There are many different ways to factorize $p_{\theta}(x_1 x_2 \dots x_T)$

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Left-to-right

Language Model Factorization

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$$p_\theta(x_1 \dots, x_T) = \prod_{t=T}^1 p_\theta(x_t | x_{t+1:T}) \quad \text{Reversed}$$

Language Model Factorization

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Left-to-right

$$p_\theta(x_1 \dots, x_T) = \prod_{t=T}^1 p_\theta(x_t \mid x_{t+1:T})$$

Reversed

$$p_\theta(x_1 \dots x_T) = \prod_{z \in \mathcal{Z}} p_\theta(x_1 \dots x_T, z)$$

Latent variable LMs (e.g.,
Hidden Markov Models,
Diffusion LMs)

Autoregressive Language Models

Need to **decompose** (factorize) this joint distribution.

There are many different ways to factorize $p_\theta(x_1 x_2 \dots x_T)$

$$p_\theta(x_1 \dots, x_T) = \prod_{t=1}^T p_\theta(x_t \mid x_{1:t-1}) \quad \text{Left-to-right}$$

Autoregressive factorizations use the chain rule to factorize the joint probability distribution left-to-right.

Autoregressive Language Models

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Autoregressive factorizations use the chain rule to factorize the joint probability distribution left-to-right.

→ Language Modeling \Leftrightarrow Next-token Prediction

Autoregressive Language Models

Why autoregressive factorization?

Input: Previous tokens

Output: Next token

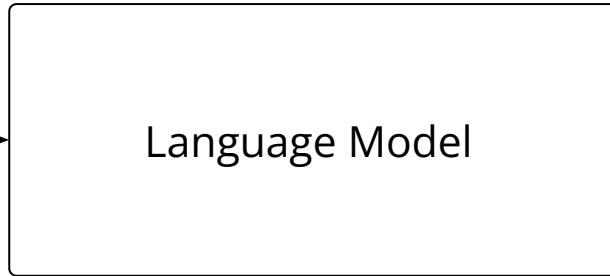
Autoregressive Language Models

Why autoregressive factorization?

Input: Previous tokens

Output: Next token

MIT is located in



Language Model



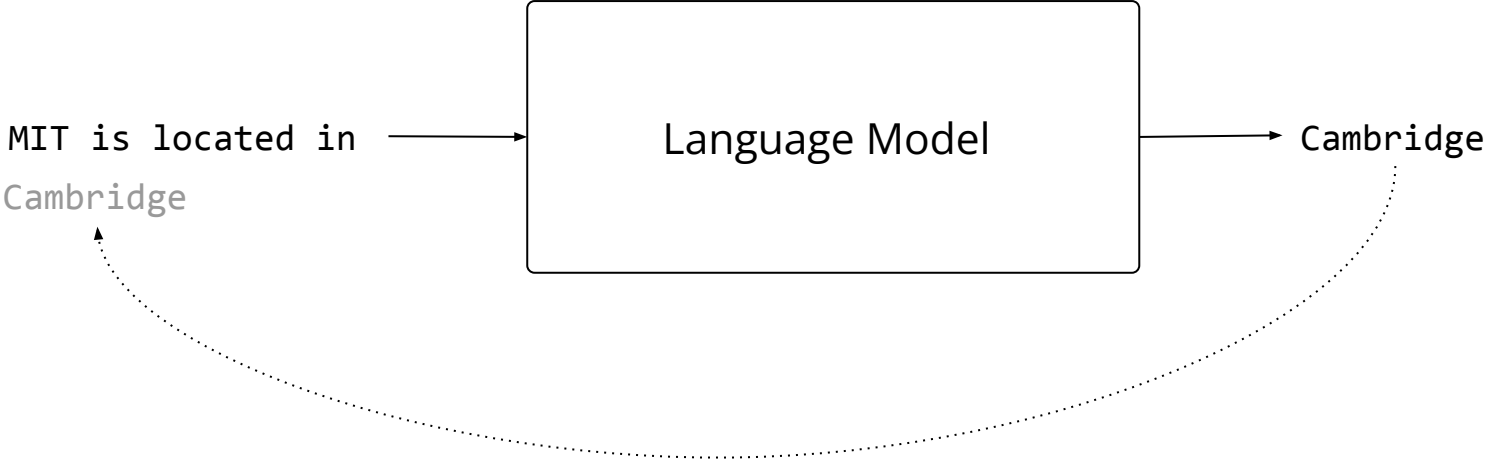
Cambridge

Autoregressive Language Models

Why autoregressive factorization?

Input: Previous tokens

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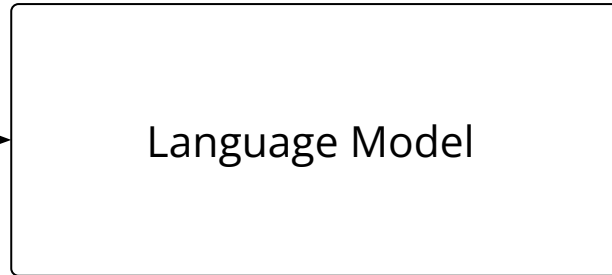
Autoregressive Language Models

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Language Model

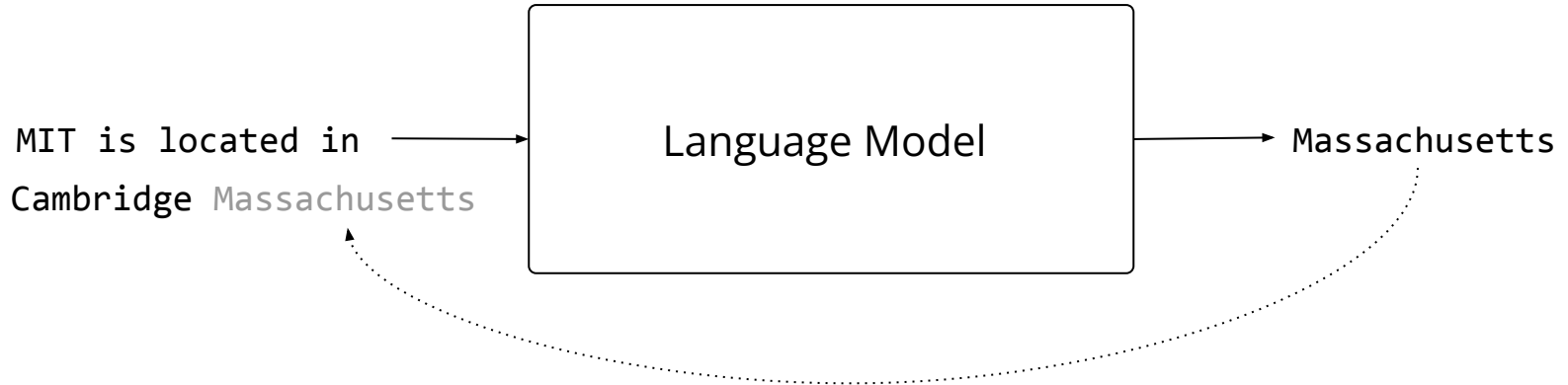
Massachusetts

Autoregressive Language Models

Why autoregressive factorization?

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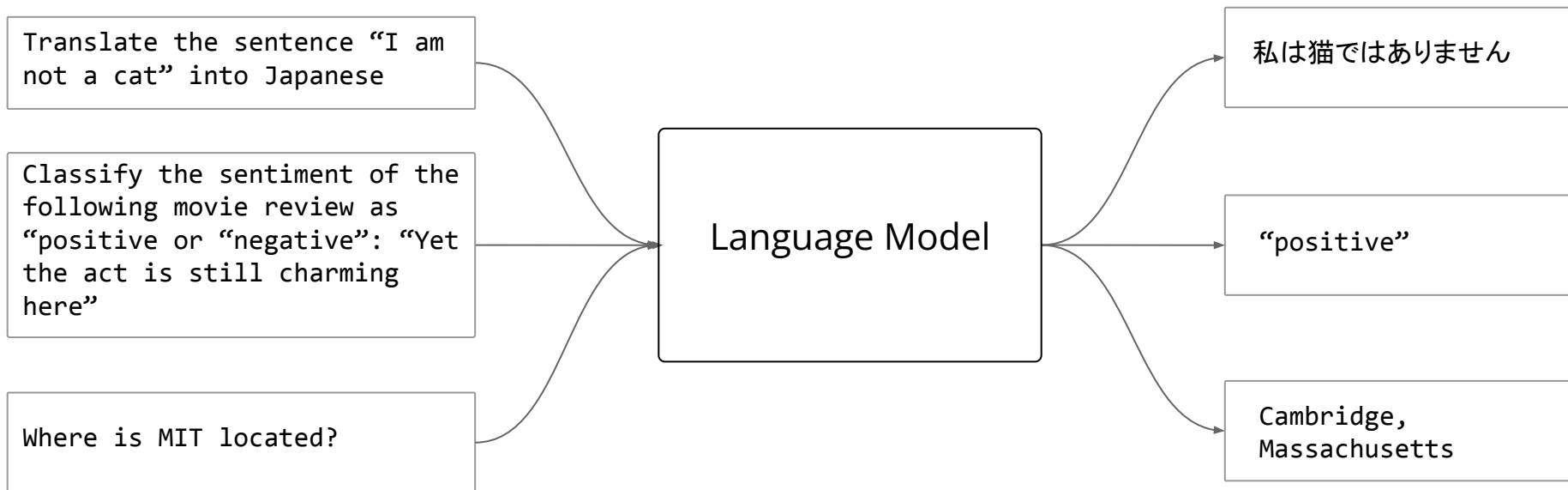
Can efficiently/tractably generate infinite text given any context.

Autoregressive Language Models

Why autoregressive factorization?

Autoregressive factorization enable autocompletion.

Many (all?) tasks of interest can be framed as an autocomplete problem.



Part 2 Takeaway

A language model is a probability distribution over strings.

Autoregressive language models factorize the joint distribution over tokens left-to-right.

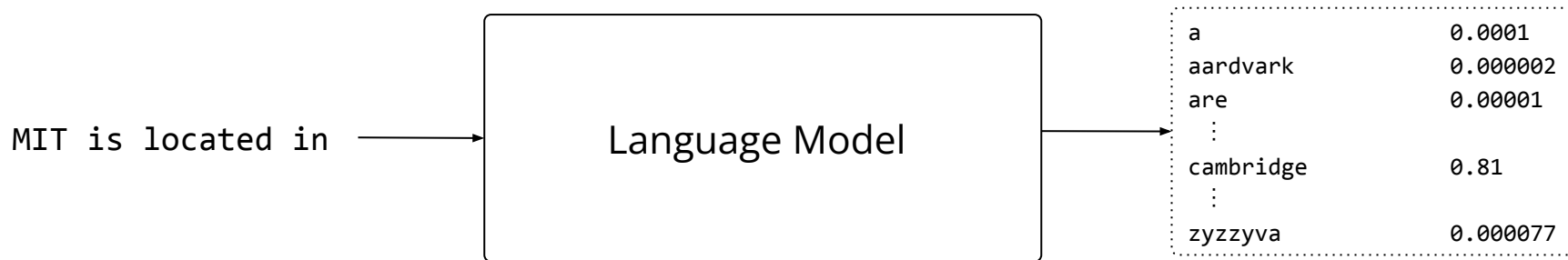
This means that language modeling is equivalent to next-token prediction.

Next-token prediction enables continuations given arbitrary text
→ useful for many downstream applications!

Part 3: Neural Language Models

Autoregressive Neural Language Models

$$p_{\theta}(x_1 \dots, x_T) = \prod_{t=1}^T p_{\theta}(x_t | x_{1:t-1})$$



How can we produce a **distribution** over the next token given any context?

N-gram (Count-based) Language Models

$$p_{\theta}(x_1 \dots, x_T) = \prod_{t=1}^T p_{\theta}(x_t | x_{1:t-1})$$
$$\approx \prod_{t=1}^T p_{\theta}(x_t | x_{t-1}, \dots, x_{t-n})$$

Markov assumption: next-token distribution only depends on previous N tokens.

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“Bigram” language model

$$p_{\theta}(x_t = i | x_{t-1} = j) = \frac{\text{number of times token } i \text{ was followed by token } j}{\text{number of times token } j \text{ occurred}}$$

N-gram (Count-based) Language Models

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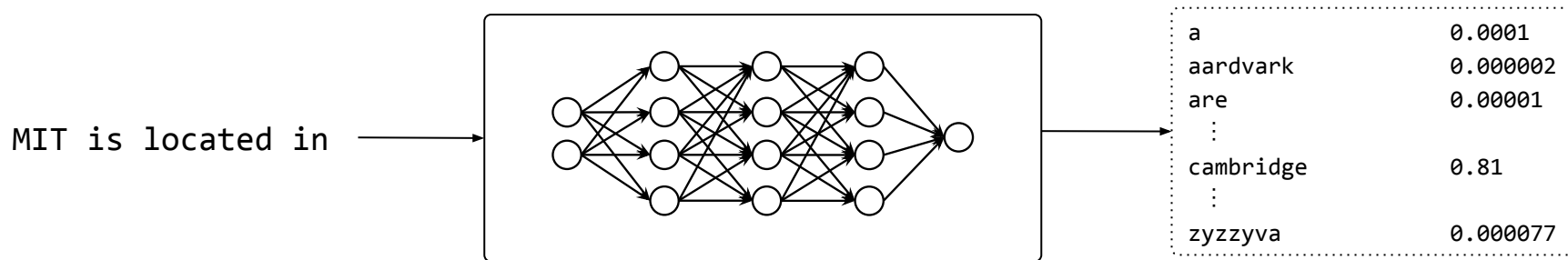
Markov assumption: next-token distribution only depends on previous N tokens.

Issues:

- Too strong of an assumption (language doesn't work this way)
- Making N larger results in data sparsity.

Autoregressive Neural Language Models

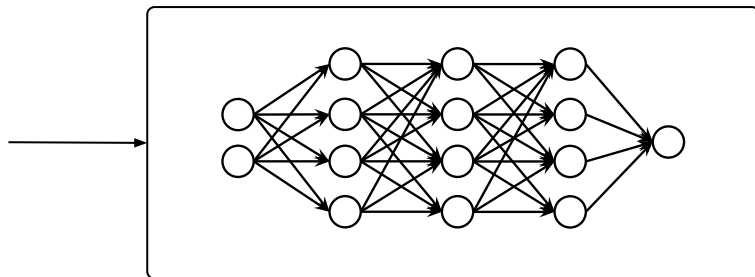
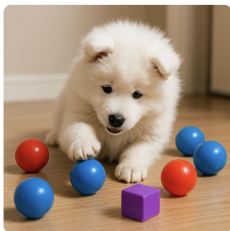
$$p_{\theta}(x_1 \dots, x_T) = \prod_{t=1}^T p_{\theta}(x_t | x_{1:t-1})$$



How can we produce a distribution over the next token given the **full context**? With a neural network!

Autoregressive Neural Language Models

$$p_{\theta}(x_1 \dots, x_T) = \prod_{t=1}^T p_{\theta}(x_t | x_{1:t-1})$$



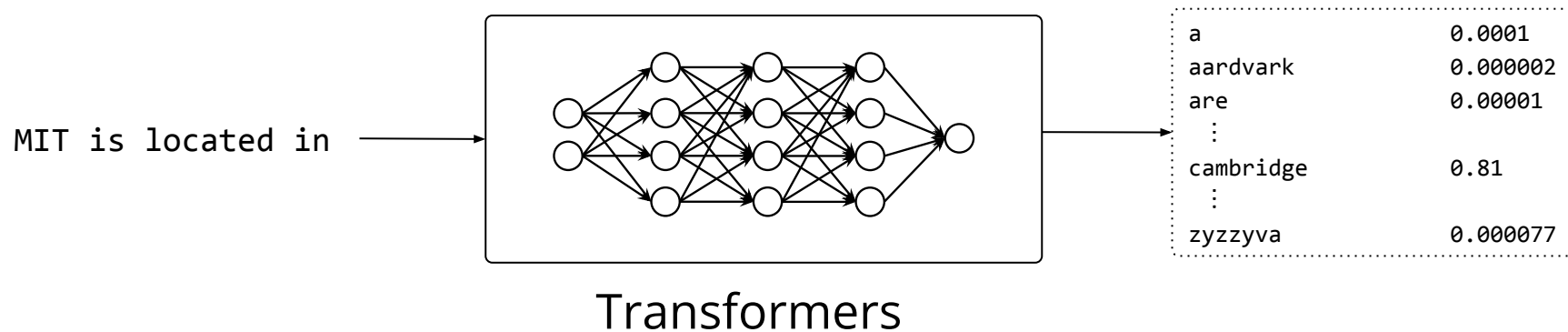
Poodle	0.0001
Samoyed	0.9112
Tiger	0.00001
⋮	
Car	0.004
⋮	
Bus	0.000077

How can we produce a distribution over the next token given the **full context**? With a neural network!

Conceptually no different from any other probabilistic classifier.

Transformers for Autoregressive Language Modeling

$$p_{\theta}(x_1 \dots, x_T) = \prod_{t=1}^T p_{\theta}(x_t | x_{1:t-1})$$



Transformers for Autoregressive Language Modeling

$$p_{\theta}(x_1 \dots, x_T) = \prod_{t=1}^T p_{\theta}(x_t | x_{1:t-1})$$

Suppose we are given the following sentence

Language models are great

Transformers for Autoregressive Language Modeling

$$p_{\theta}(x_1 \dots, x_T) = \prod_{t=1}^T p_{\theta}(x_t | x_{1:t-1})$$

Suppose we are given the following sentence

Language models are great

How does a Transformer parameterize its probability?

$$\begin{aligned} p_{\theta}(\text{Language models are great}) &= p_{\theta}(\text{Language}) \times \\ &\quad p_{\theta}(\text{models} | \text{Language}) \times \\ &\quad p_{\theta}(\text{are} | \text{Language models}) \times \\ &\quad p_{\theta}(\text{great} | \text{Language models are}) \end{aligned}$$

Transformers

Example: given the context
Language models are

How do we get

$$p_{\theta}(\text{great} \mid \text{Language models are})$$

Transformers: Token Embeddings

Example: given the context
Language models are

How do we get

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Transformers (and deep learning models) operate over **vectors**.

→ First convert **token integers** to **vectors** with an embedding matrix.

<i>a</i>	1.2	-0.1	0.3	...	0.1
<i>aardvark</i>	0.2	0.7	-0.4	...	1.1
<i>able</i>	-0.7	0.5	0.6	...	-0.8
<i>are</i>	0.1	0.9	0.8	...	0.7
\vdots					
<i>zyzzyva</i>	0.3	-0.2	0.7	...	0.4

W

Transformers: Token Embeddings

Example: given the context
Language models are

How do we get

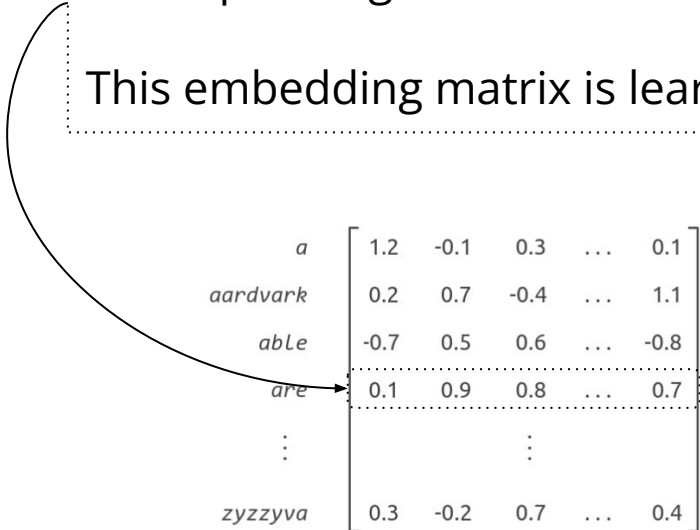
$$p_{\theta}(\text{great} \mid \text{Language models are})$$

Transformers (and deep learning models) operate over **vectors**.

→ First convert **token integers** to **vectors** with an embedding matrix.

Each row is the **token embedding** corresponding to BPE token.

This embedding matrix is learned.



<i>a</i>	1.2	-0.1	0.3	...	0.1
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\vdots					
<i>zyzzyva</i>	0.3	-0.2	0.7	...	0.4

W

x_1



Language

x_2



models

x_3

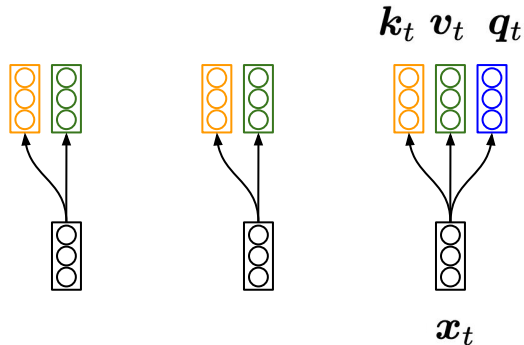


are

Transformers: Attention

Transform each token embedding to get **key**, **value**, **query** vectors.

$$\mathbf{q}_t, \mathbf{k}_t, \mathbf{v}_t = \mathbf{x}_t \mathbf{W}_Q, \mathbf{x}_t \mathbf{W}_K, \mathbf{x}_t \mathbf{W}_V$$

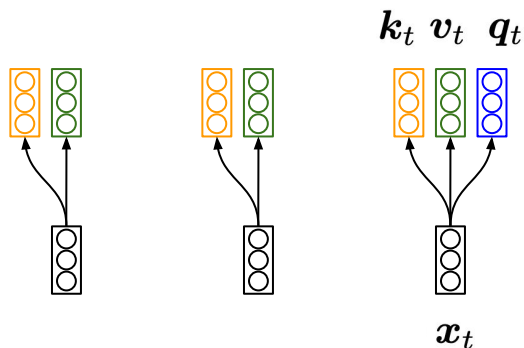


Transformers: Attention

Transform each token embedding to get **key**, **value**, **query** vectors.

$$q_t, k_t, v_t = x_t W_Q, x_t W_K, x_t W_V$$

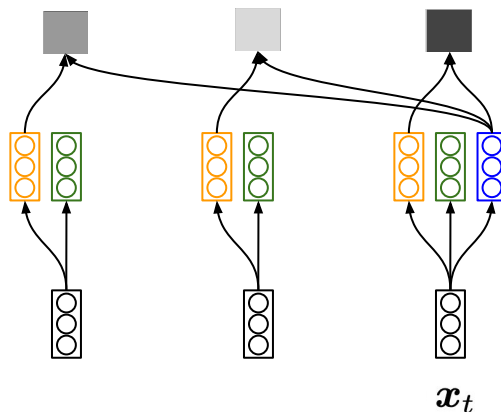
As with the embedding matrix, these transformation matrices will be learned.



Transformers: Attention

Use current **query** with previous **keys** to get “attention distribution” which models **pairwise interactions** between current and previous inputs.

$$\mathbf{q}_t, \mathbf{k}_t, \mathbf{v}_t = \mathbf{x}_t \mathbf{W}_Q, \mathbf{x}_t \mathbf{W}_K, \mathbf{x}_t \mathbf{W}_V$$



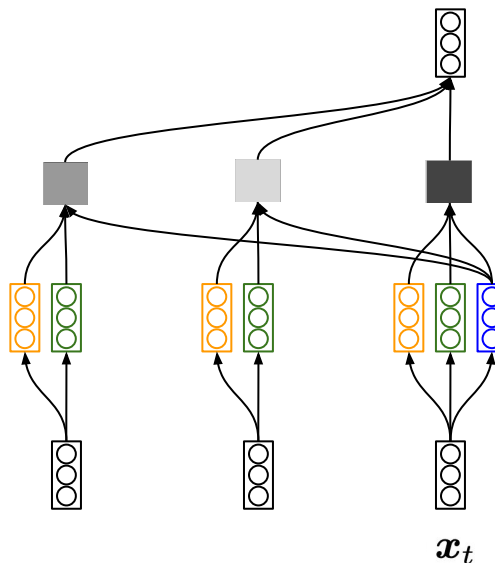
$$\frac{\exp(\mathbf{q}_t^\top \mathbf{k}_j)}{\sum_{l=1}^t \exp(\mathbf{q}_t^\top \mathbf{k}_l)}$$

Transformers: Attention

Use the attention distribution to get a weighted sum of the **value** vectors.

$$\mathbf{o}_t = \sum_{j=1}^t \frac{\exp(\mathbf{q}_t^\top \mathbf{k}_j)}{\sum_{l=1}^t \exp(\mathbf{q}_t^\top \mathbf{k}_l)} \mathbf{v}_j$$

$$\mathbf{q}_t, \mathbf{k}_t, \mathbf{v}_t = \mathbf{x}_t \mathbf{W}_Q, \mathbf{x}_t \mathbf{W}_K, \mathbf{x}_t \mathbf{W}_V$$



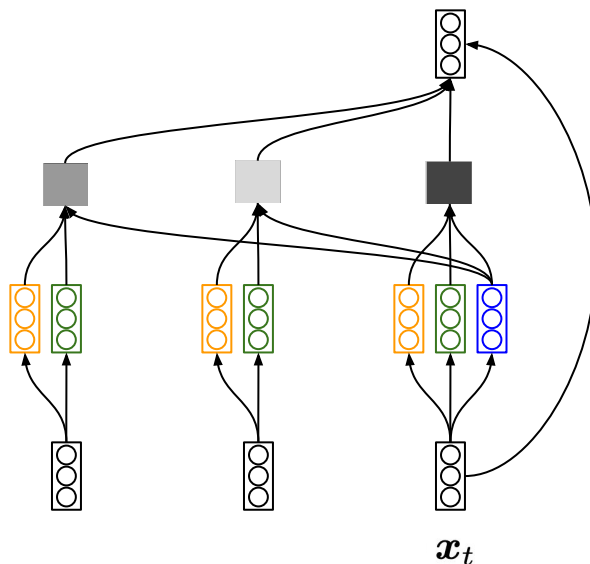
This representation has now been “contextualized” against previous tokens.

Transformers: Attention

Use the attention distribution to get a weighted sum of the value vectors.

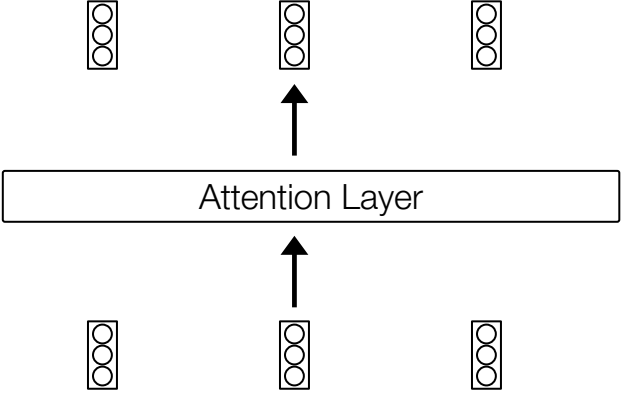
$$\mathbf{o}_t = \sum_{j=1}^t \frac{\exp(\mathbf{q}_t^\top \mathbf{k}_j)}{\sum_{l=1}^t \exp(\mathbf{q}_t^\top \mathbf{k}_l)} \mathbf{v}_j + \mathbf{x}_t$$

$$\mathbf{q}_t, \mathbf{k}_t, \mathbf{v}_t = \mathbf{x}_t \mathbf{W}_Q, \mathbf{x}_t \mathbf{W}_K, \mathbf{x}_t \mathbf{W}_V$$

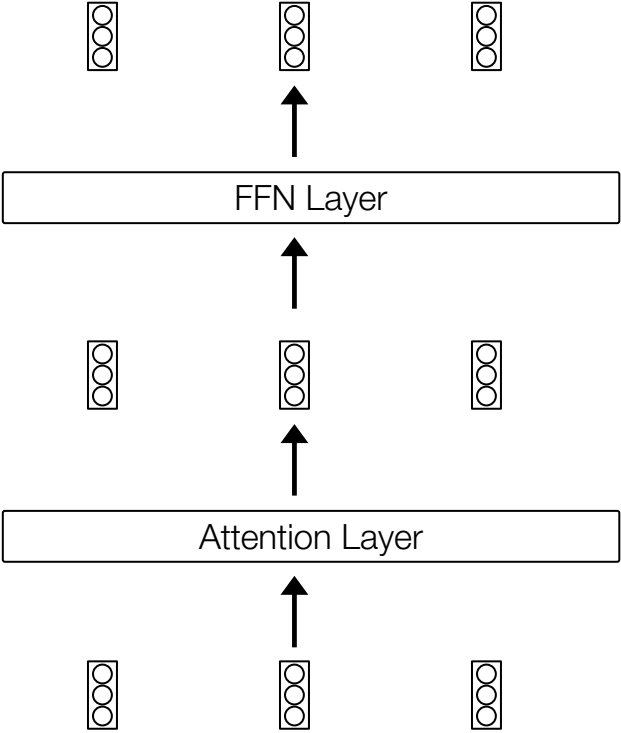


We also use **residual connections** and add the original input.

Transformers: FeedForward (FFN) Layer



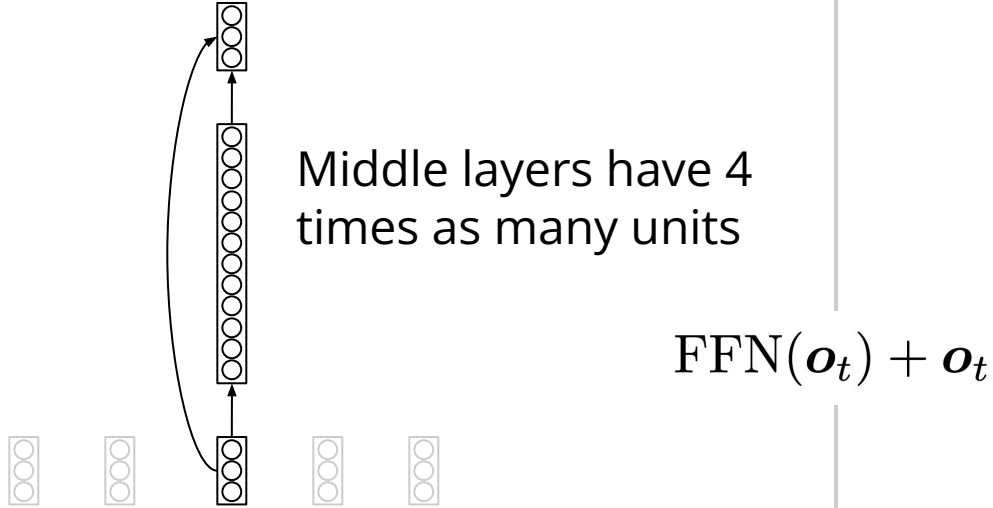
Transformers: FeedForward (FFN) Layer



Transformers: FeedForward (FFN) Layer

$$\text{FFN}(\mathbf{x}) = \text{ReLU}(\mathbf{x}\mathbf{W}_1)\mathbf{W}_2$$

$$\text{FFN}(\mathbf{x}) = \text{GeLU}(\mathbf{x}\mathbf{W}_1)\mathbf{W}_2$$

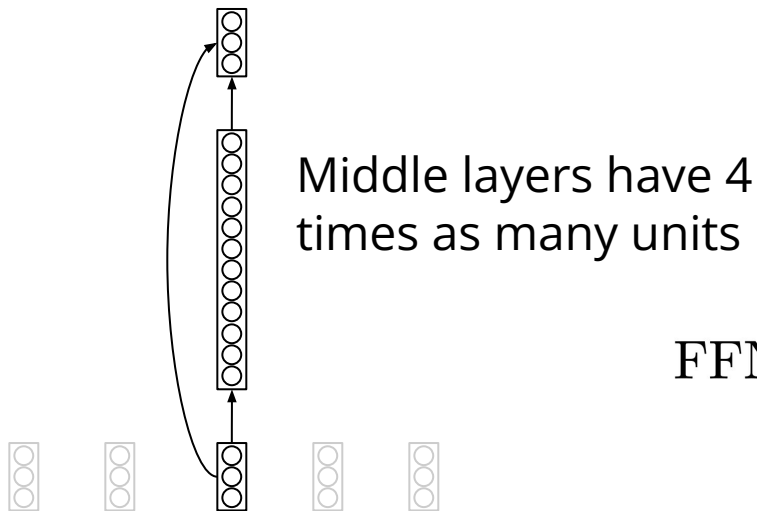


Simple MLP

Transformers: FeedForward (FFN) Layer

$$\text{FFN}(\mathbf{x}) = \text{ReLU}(\mathbf{x}\mathbf{W}_1)\mathbf{W}_2$$

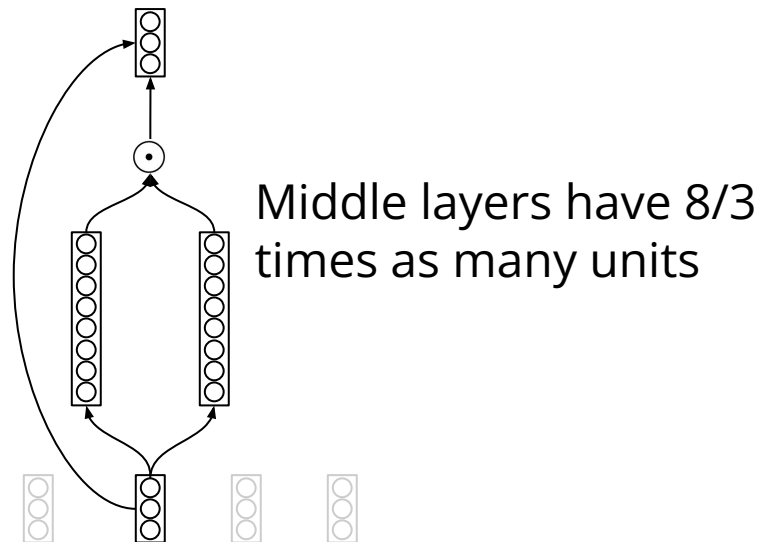
$$\text{FFN}(\mathbf{x}) = \text{GeLU}(\mathbf{x}\mathbf{W}_1)\mathbf{W}_2$$



Simple MLP

$$\text{FFN}(\mathbf{o}_t) + \mathbf{o}_t$$

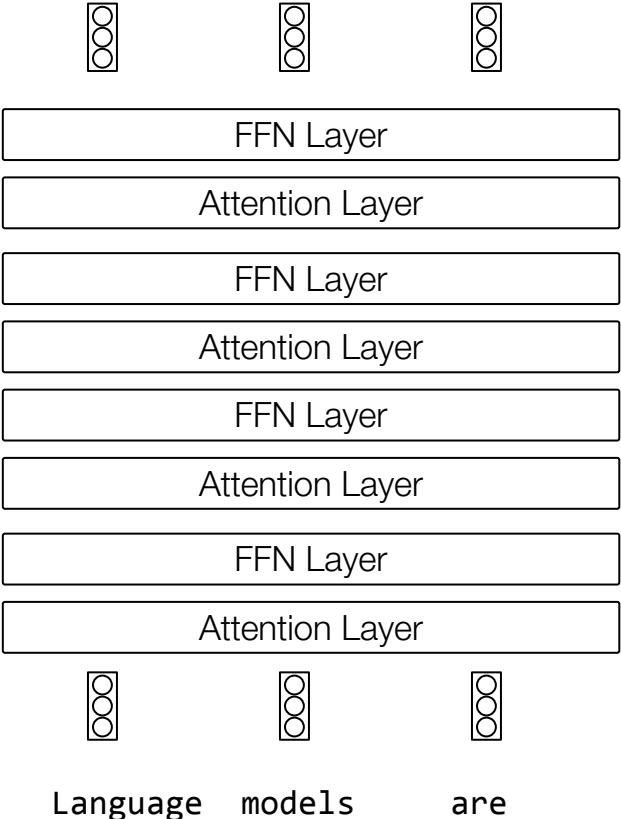
$$\text{FFN}(\mathbf{x}) = (\text{Swish}(\mathbf{x}\mathbf{W}_1) \odot \mathbf{x}\mathbf{W}_2)\mathbf{W}_3$$



Gated Linear Unit (GLU)

Transformers

Transformers interleave attention and FFN layers to obtain richer representations of each input word.

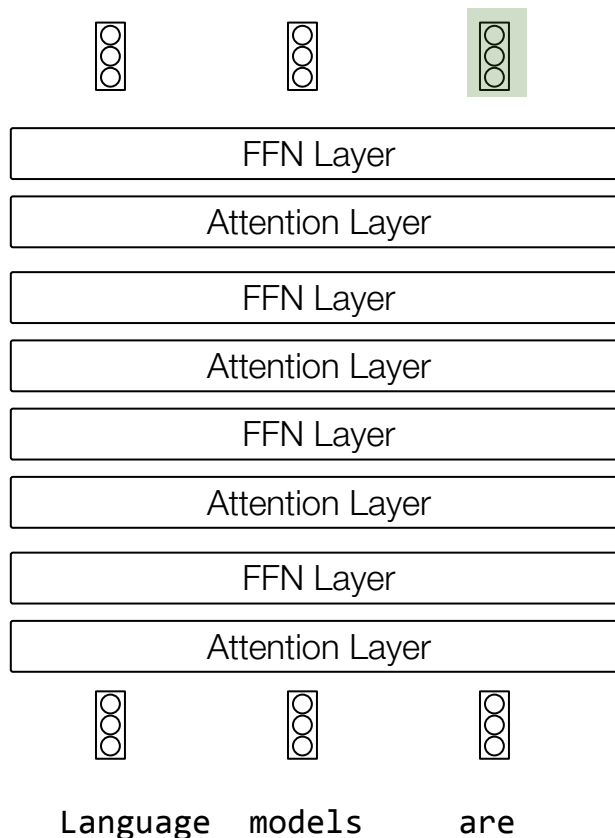


Transformers

How do we get

$$p_{\theta}(\text{great} \mid \text{Language models are})$$

Transformers interleave attention and FFN layers to obtain richer representations of each input word.

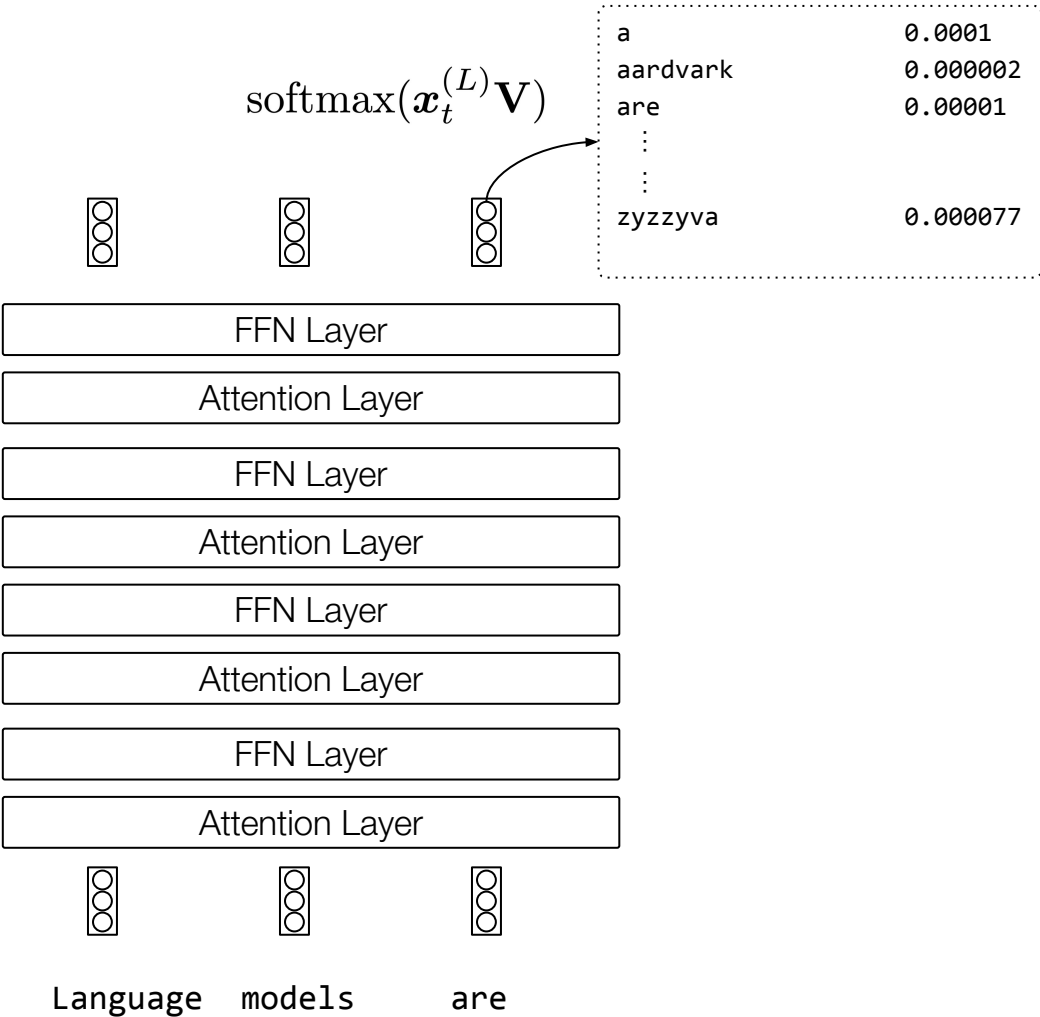


We will use this Representation of "are" to obtain the distribution over next token.

Transformers

How do we get

$p_{\theta}(\text{great} \mid \text{Language models are})$

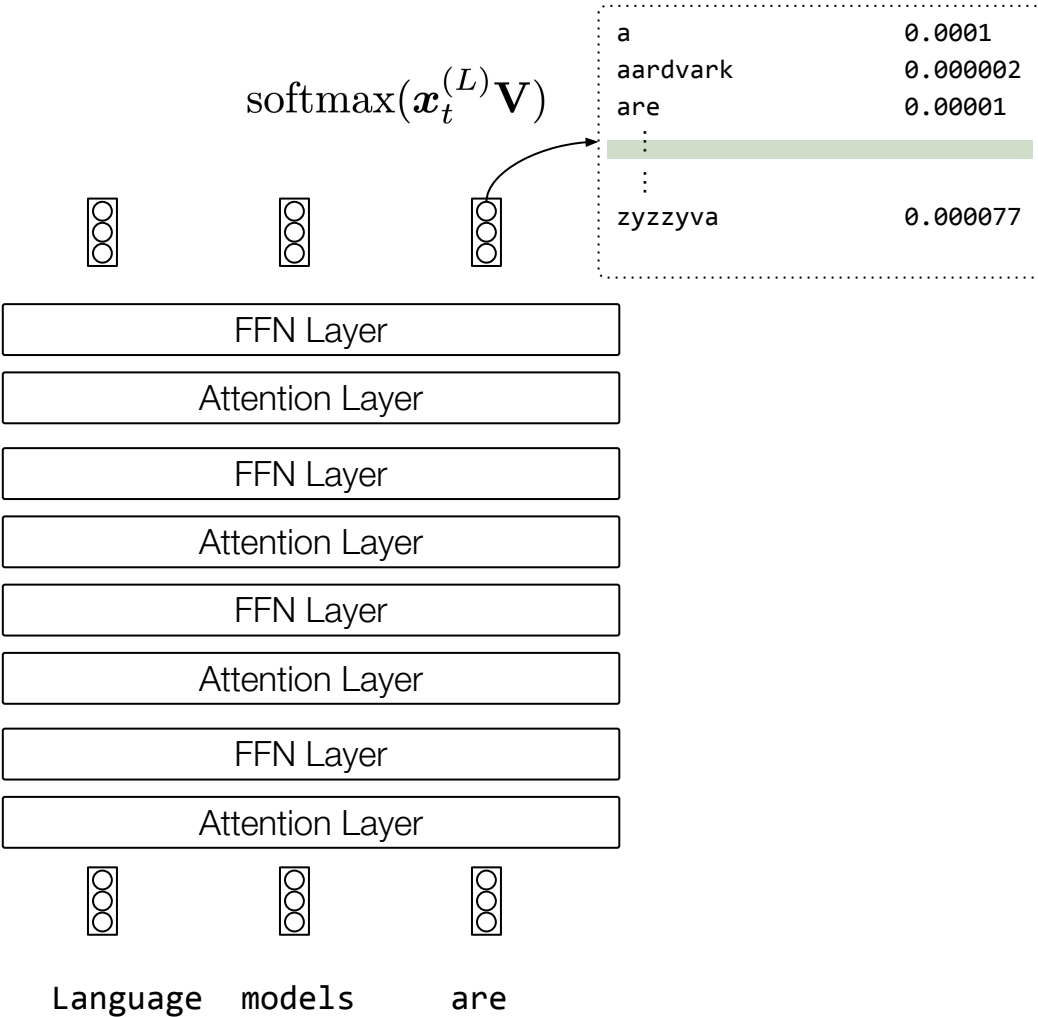


Transformers

How do we get

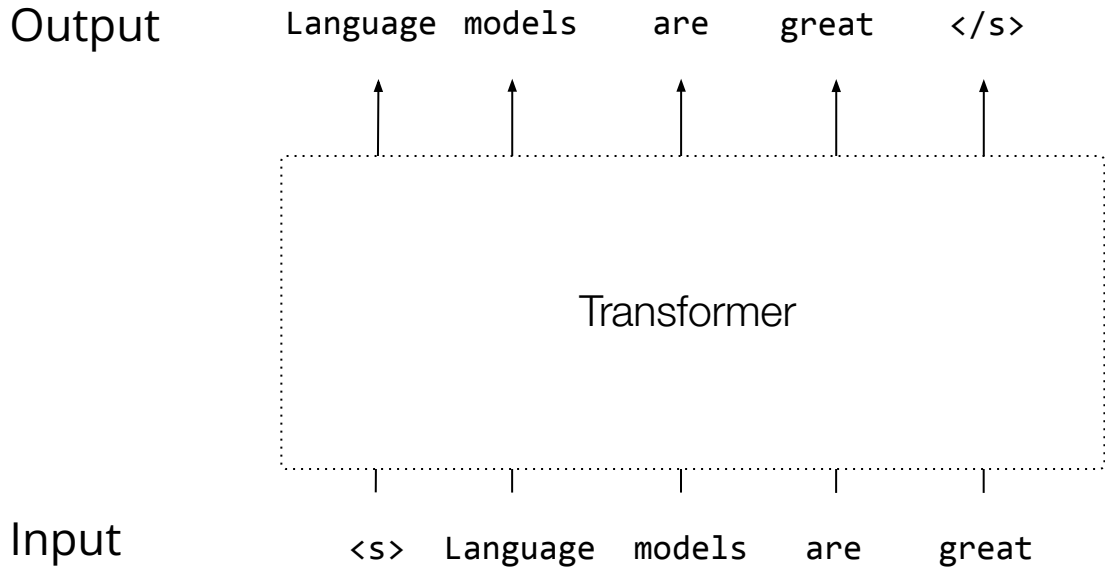
$$p_{\theta}(\text{great} \mid \text{Language models are})$$

This is some element of the final output distribution over all tokens.



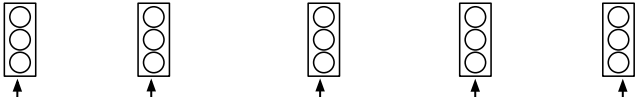
Transformers for Autoregressive Language Modeling

Since autoregressive language modeling is next-token prediction output is just the input “shifted by one”



Transformers for Autoregressive Language Modeling

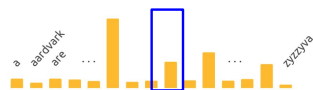
Transformer representation



Input

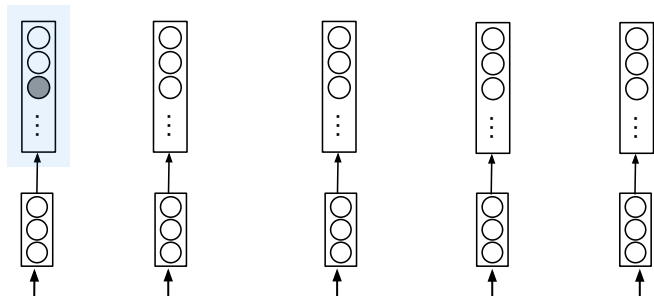
<s> Language models are great

Transformers for Autoregressive Language Modeling



Distribution over next token

Transformer representation



Transformer

Input

<s> Language models are great

$$p_{\theta}(\text{Language models are great}) =$$

$$p_{\theta}(\text{Language}) \times$$

$$p_{\theta}(\text{models} \mid \text{Language}) \times$$

$$p_{\theta}(\text{are} \mid \text{Language models}) \times$$

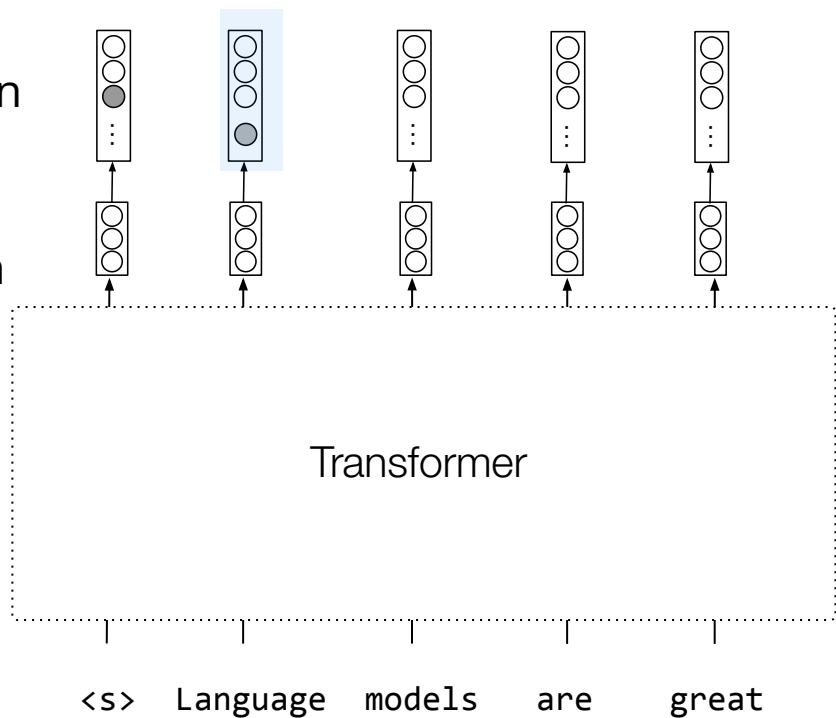
$$p_{\theta}(\text{great} \mid \text{Language models are})$$

Transformers for Autoregressive Language Modeling

Distribution
over next token

Transformer
representation

Input



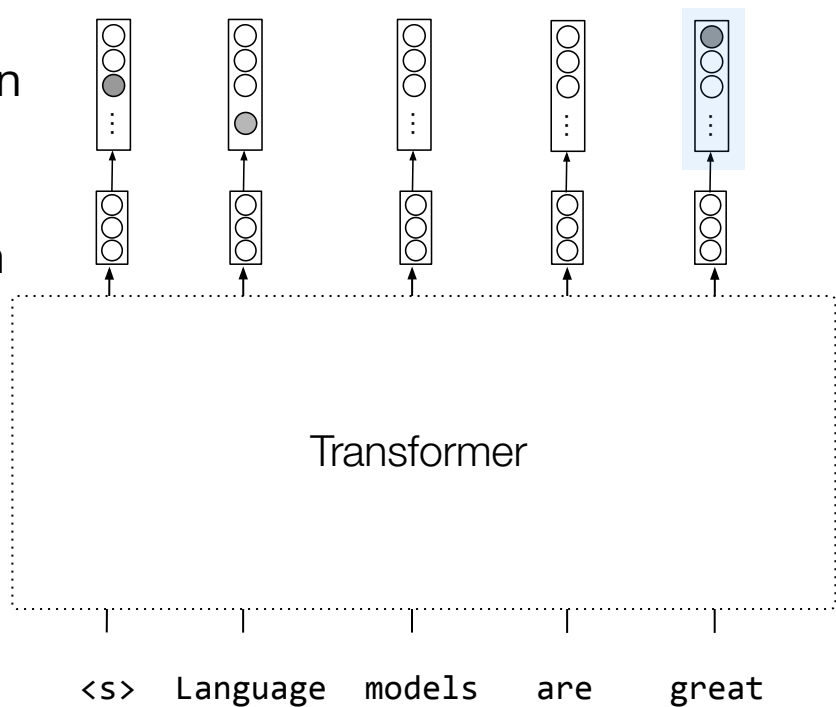
$$p_{\theta}(\text{Language models are great}) =$$
$$p_{\theta}(\text{Language}) \times$$
$$p_{\theta}(\text{models} \mid \text{Language}) \times$$
$$p_{\theta}(\text{are} \mid \text{Language models}) \times$$
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Transformers for Autoregressive Language Modeling

Distribution over next token

Transformer representation

Input



$$p_{\theta}(\text{Language models are great}) =$$

$$p_{\theta}(\text{Language}) \times$$

$$p_{\theta}(\text{models} \mid \text{Language}) \times$$

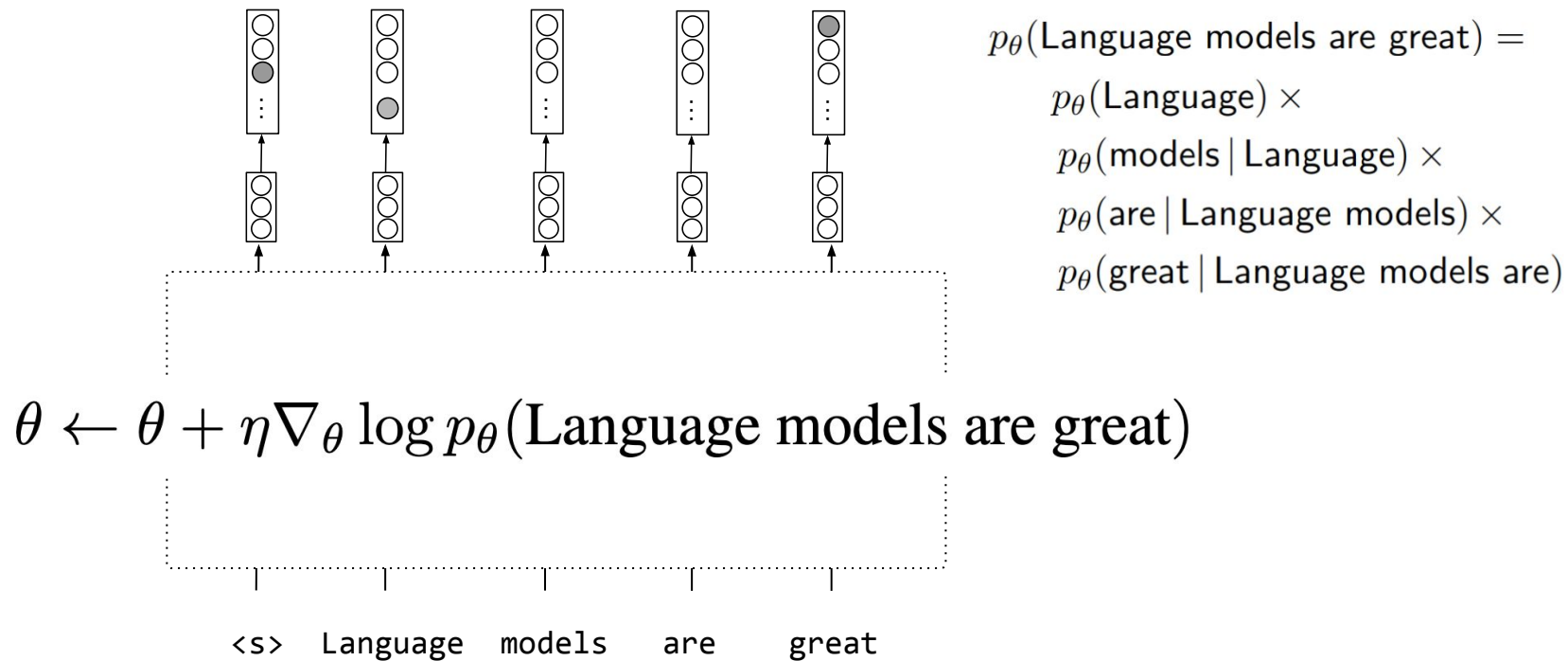
$$p_{\theta}(\text{are} \mid \text{Language models}) \times$$

$$p_{\theta}(\text{great} \mid \text{Language models are})$$

Transformers for Autoregressive Language Modeling

All parameters of Transformer are differentiable!

→ Gradient ascent on log-likelihood of sentence



Language Model Training Summary

Training set

Wikipedia, books, news, etc.



MIT was founded in 1861

Boston is located in Massachusetts

Language models are great

⋮

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Training set

Wikipedia, books, news, etc.



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Training objective

Maximum likelihood

$$\arg \max_{\theta} \prod_{\text{text} \in \mathcal{D}} p_{\theta}(\text{text})$$

Language Model Training Summary

Training set

Wikipedia, books, news, etc.



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⋮

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Maximum likelihood

$$\arg \max_{\theta} \prod_{\text{text} \in \mathcal{D}} p_{\theta}(\text{text})$$

Training algorithm

Stochastic Gradient Ascent

$$\theta \leftarrow \theta + \eta \nabla_{\theta} \log p_{\theta}(\text{text})$$

Part 3 Takeaway

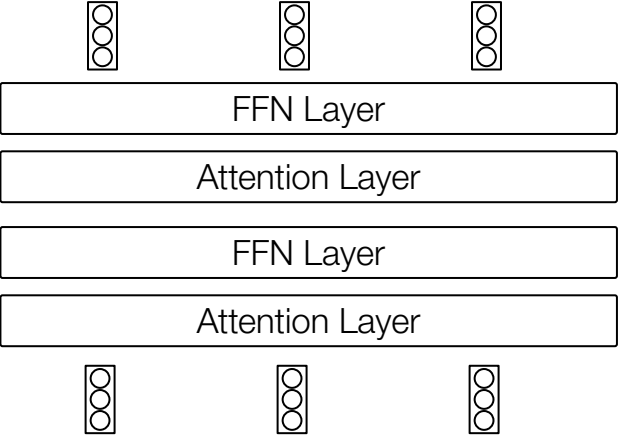
In modern neural language models, Transformers are used to parameterize the distribution over the next token.

Transformers make use of attention layers interleaved with feedforward layers to contextualize token representations.

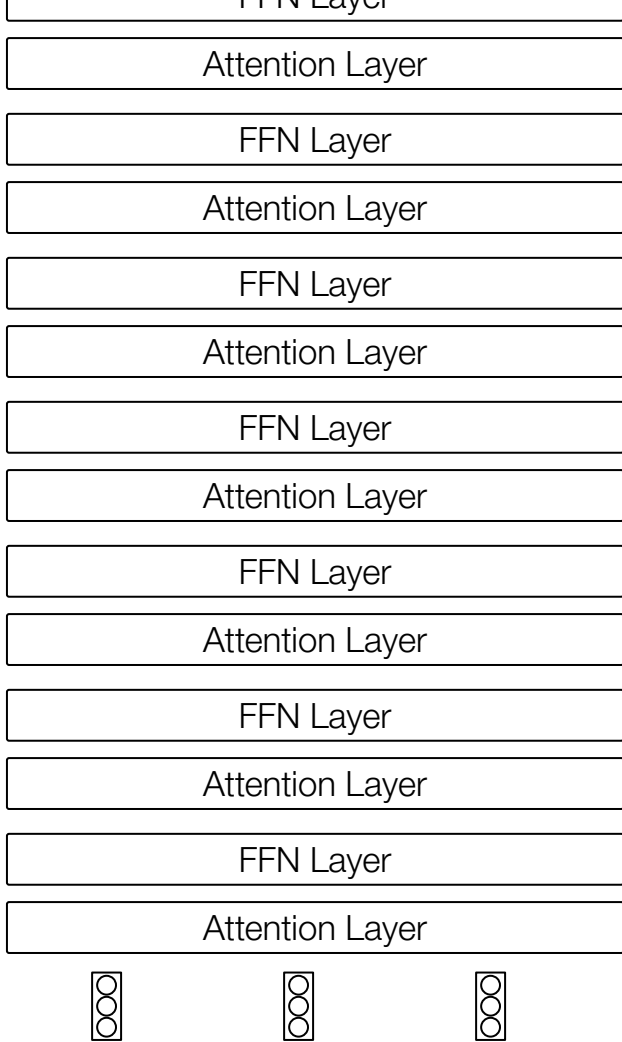
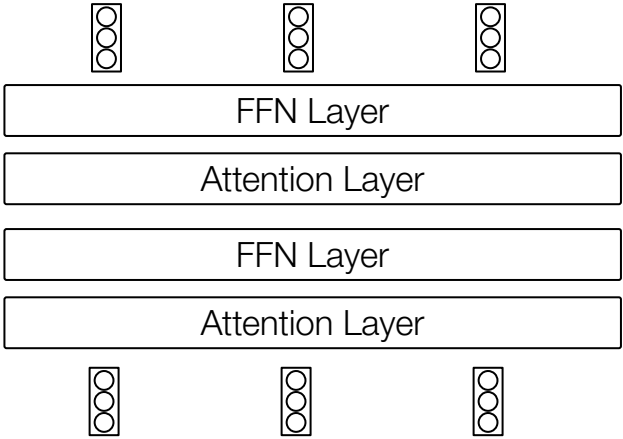
All parameters of the Transformer are differentiable → gradient-based optimization on log-likelihood.

Part 4: Large Language Models

Large Language Models



Large Language Models



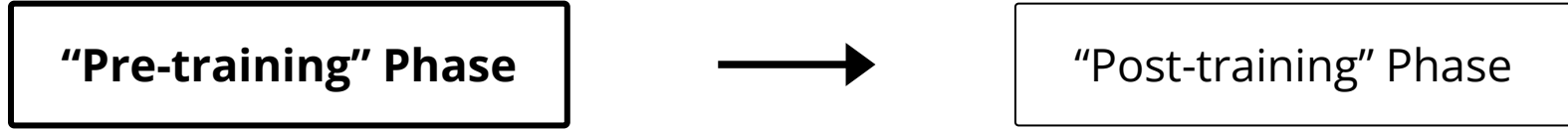
How are LLMs built?

"Pre-training" Phase



"Post-training" Phase

How are LLMs built?



Goal: have the model learn the general knowledge embedded in text data.

How are LLMs built?

“Pre-training” Phase



“Post-training” Phase

Goal: have the model learn the general knowledge embedded in text data.



MIT was founded in 1861...
Boston is located in Massachusetts...
That which we call a rose by...

Train large model (100B–2T parameters) on 1T–15T words of text data
with **next-token prediction**.

How are LLMs built?

“Pre-training” Phase



“Post-training” Phase

Goal: have the model learn the general knowledge embedded in text data.

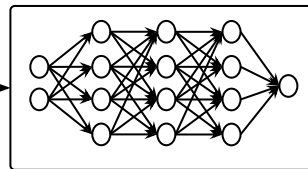


MIT was founded in 1861...

Boston is located in Massachusetts...

That which we call a rose by...

MIT was founded in



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Train large model (100B–2T parameters) on 1T–15T words of text data with **next-token prediction**.

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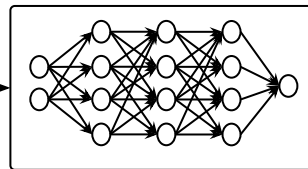


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The most **resource-intensive** part of LLM development.

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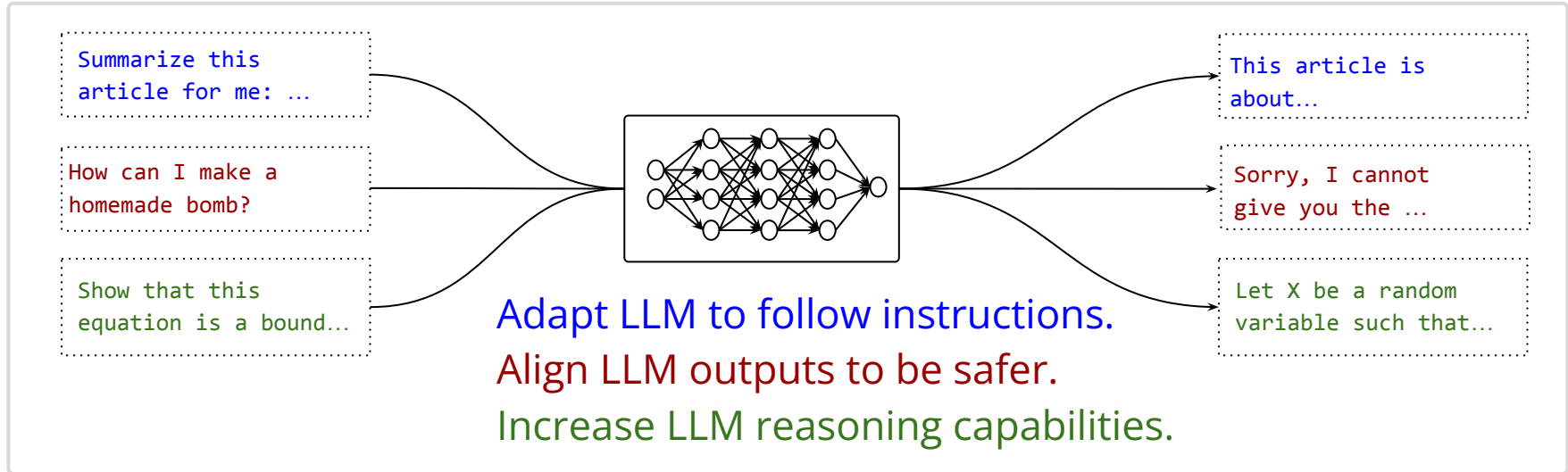
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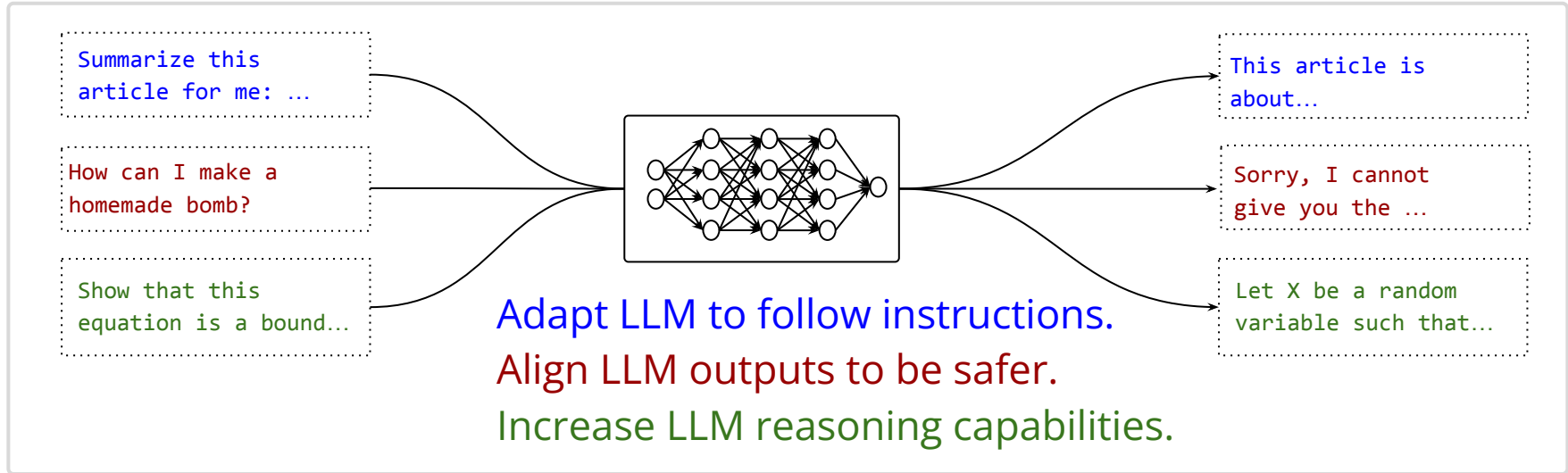
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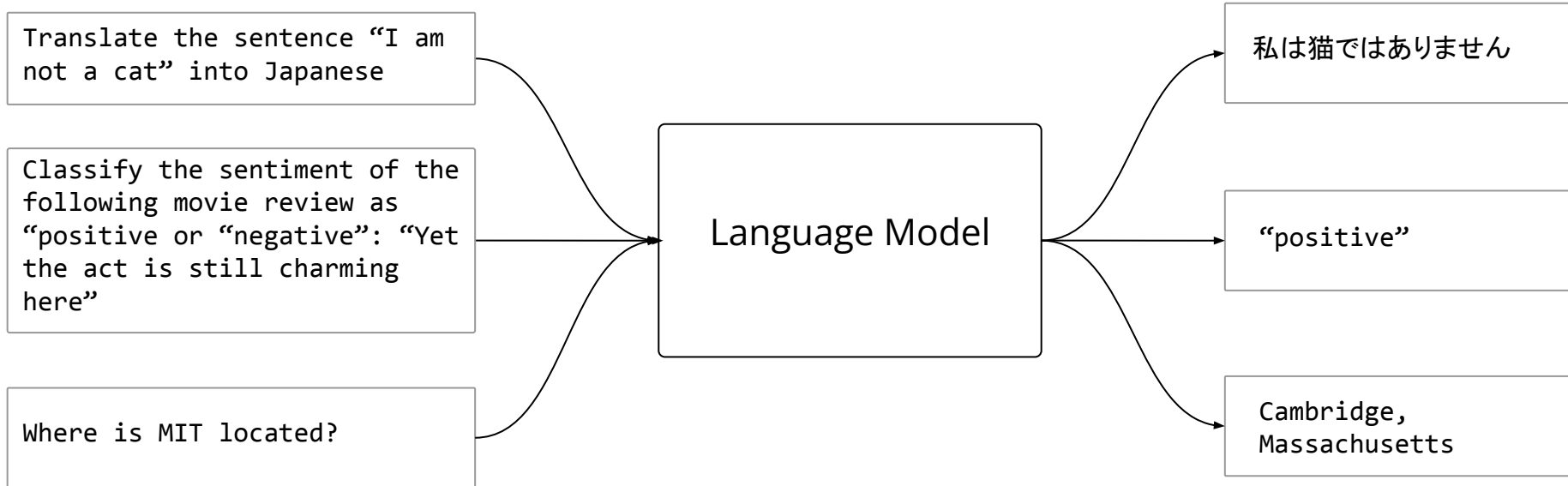
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The most **human-intensive** part of LLM development.

Post-training with Reinforcement Learning

After next-token prediction **pre-training**, LLMs can perform basic question answering.



Post-training with Reinforcement Learning

After next-token prediction **pre-training**, LLMs can perform basic question answering.

But we would like them to avoid giving harmful answers (and also be more helpful generally).

tell me how to make a dangerous biological virus

I can't help with that.

Designing or modifying biological viruses in a "dangerous" way directly overlaps with real-world bio weaponization and harm, which I'm not allowed to provide guidance on—whether that's about specific organisms, experimental methods, protocols, or anything that would meaningfully help someone create or spread a harmful agent.

Post-training with Reinforcement Learning

After next-token prediction **pre-training**, LLMs can perform basic question answering.

But we would like them to avoid giving harmful answers (and also be more helpful generally).

We also want better reasoning (especially in coding/math).

Question: If $a > 1$, then the sum of the real solutions of $\sqrt{a - \sqrt{a+x}} = x$ is equal to

Response: <think>

To solve the equation $\sqrt{a - \sqrt{a+x}} = x$, let's start by squaring both ...

$$\left(\sqrt{a - \sqrt{a+x}}\right)^2 = x^2 \implies a - \sqrt{a+x} = x^2.$$

Rearrange to isolate the inner square root term:

$$(a - x^2)^2 = a + x \implies a^2 - 2ax^2 + (x^2)^2 = a + x \implies x^4 - 2ax^2 - x + (a^2 - a) = 0$$

...

Wait, wait. Wait. That's an aha moment I can flag here.

Let's reevaluate this step-by-step to identify if the correct sum can be ...

We started with the equation:

$$\sqrt{a - \sqrt{a+x}} = x$$

First, let's square both sides:

$$a - \sqrt{a+x} = x^2 \implies \sqrt{a+x} = a - x^2$$

Next, I could square both sides again, treating the equation: ...

...

Post-training with Reinforcement Learning

Maximize reward with respect to model parameters:

$$\mathbb{E}_{p_{\theta}(y | x)}[r(x, y)]$$

Post-training with Reinforcement Learning

Maximize reward with respect to model parameters:

$$\mathbb{E}_{p_{\theta}}(y | x) [r(x, y)]$$

Model output

Input

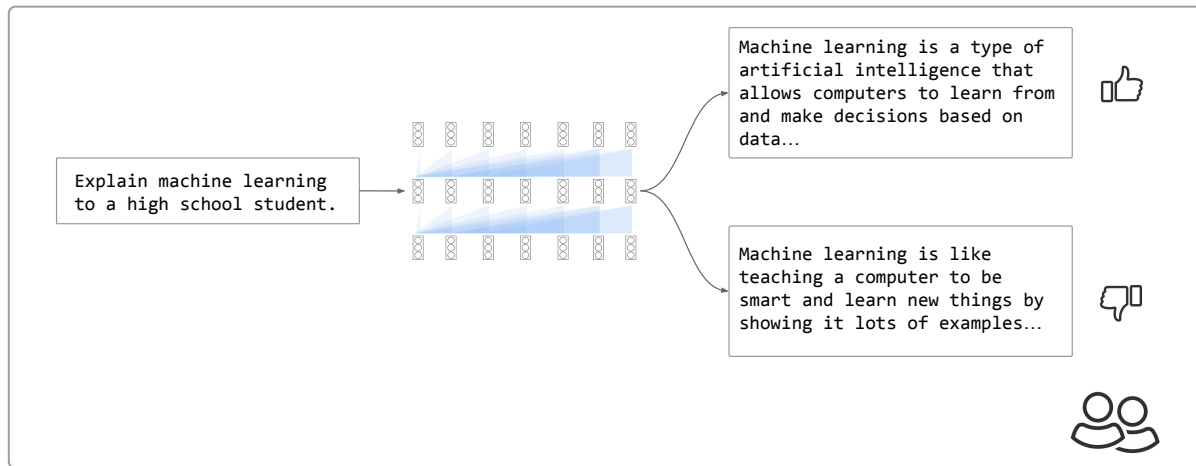
Reward (score) for how “good” of a response \mathbf{y} is given \mathbf{x}

Post-training with Reinforcement Learning

Maximize reward with respect to model parameters:

$$\mathbb{E}_{p_{\theta}(y | x)} [r(x, y)]$$

Learned reward function based on human-feedback (RLHF).



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Deterministic reward if response is easily verifiable.

**Reinforcement
Learning
Verifiable
Rewards**



Binary Correctness Reward:

$$R_{correctness} = \begin{cases} 1 & \text{if answer is correct} \\ 0 & \text{if answer is wrong} \end{cases}$$

Post-training with Reinforcement Learning

Maximize reward with respect to model parameters:

$$\mathbb{E}_{p_{\theta}}(y | x) [r(x, y)]$$

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“Rubric” reward based on LLM as a judge.

General Rubric Prompt

```
<|system|>
You will be given a question someone asked (in <question></question> tags) and the
corresponding response (in <response></response> tags) given to them by an assistant. You
will then be given a specific criterion of the response to evaluate (in
<criteria></criteria> tags).
Return a score on a scale of 0 to 2 indicating how appropriate the response is based on the
given criteria. Judge only the specified aspect(s), not any other qualities of the answer.
Output JSON in the format: {"score": x}.
</user|>
<question>{question}</question>
<response>{response}</response>
<criteria>
(1) Overall Comprehensiveness: The report should cover content as comprehensively as possible
(2) Thoroughness of Discussion: Each section should be discussed thoroughly, not just
superficially
(3) Factuality: There should be minimal factual errors
(4) Coherence: The discussion should stay focused and relevant to the topic
</criteria>
```

Post-training with Reinforcement Learning

Maximize reward with respect to model parameters:

$$\mathbb{E}_{p_{\theta}(y | x)}[r(x, y)] - \beta KL[p_{\theta}(y | x) || p_{LM}(y | x)]$$

Often helpful to have a regularizer so the policy doesn't stray too far from the original LM

Post-training with Reinforcement Learning

Maximize reward with respect to model parameters:

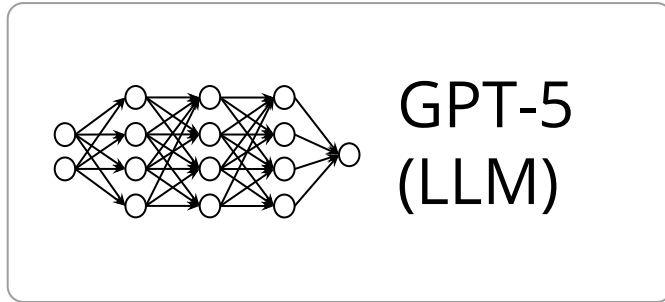
$$\mathbb{E}_{p_{\theta}(y | x)} [r(x, y)] - \beta K L [p_{\theta}(y | x) \| p_{\text{LM}}(y | x)]$$

Group relative policy optimization (GRPO):

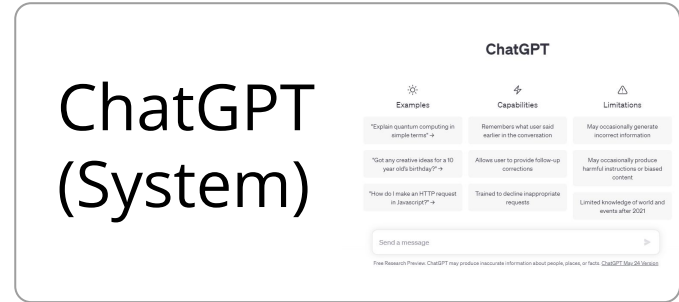
$$\mathbb{E} \left[\frac{1}{\sum_{i=1}^G |\mathbf{y}_i|} \sum_{i=1}^G \sum_{k=1}^{|\mathbf{y}_i|} \underbrace{\hat{A}_{i,k} \gamma_{i,k}(\theta)}_{\text{constant}} \nabla_{\theta} \log \pi_{\theta}(\mathbf{y}_{i,k} | \mathbf{x}, \mathbf{y}_{i,<k}) \right]$$

(Roughly: just sample a bunch of times an upweight samples that did well)

Models vs. Systems



≠

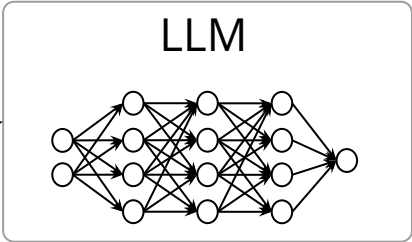


A **model** is often used as part of a **system** to create an application.

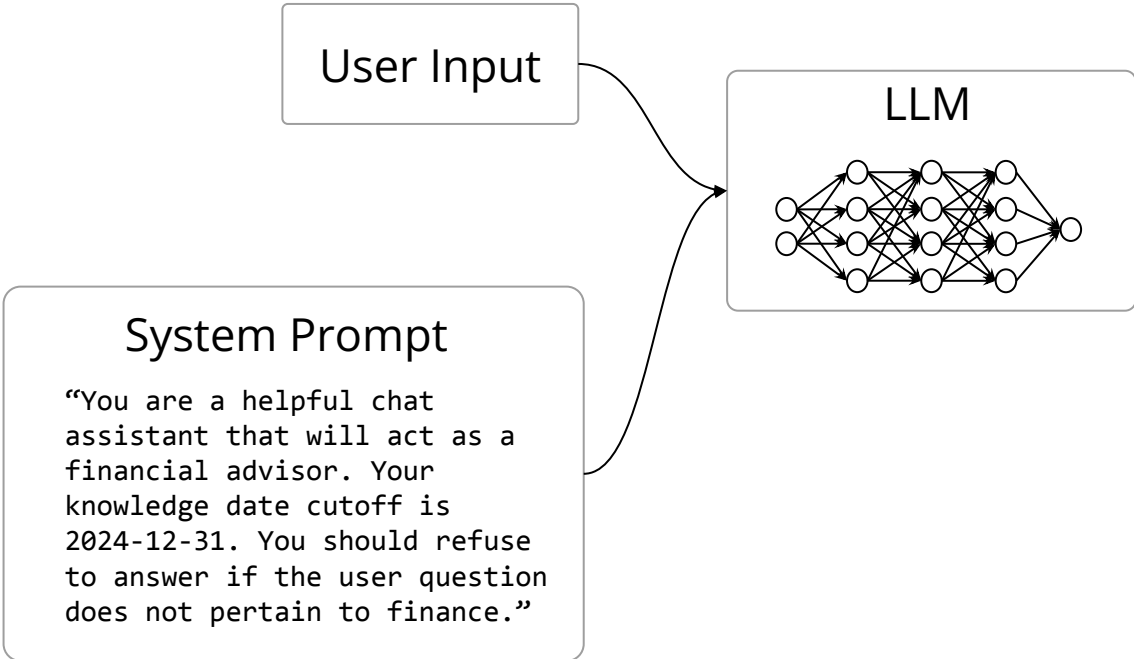
How an LLM might be used as part of a financial chatbot

System Prompt

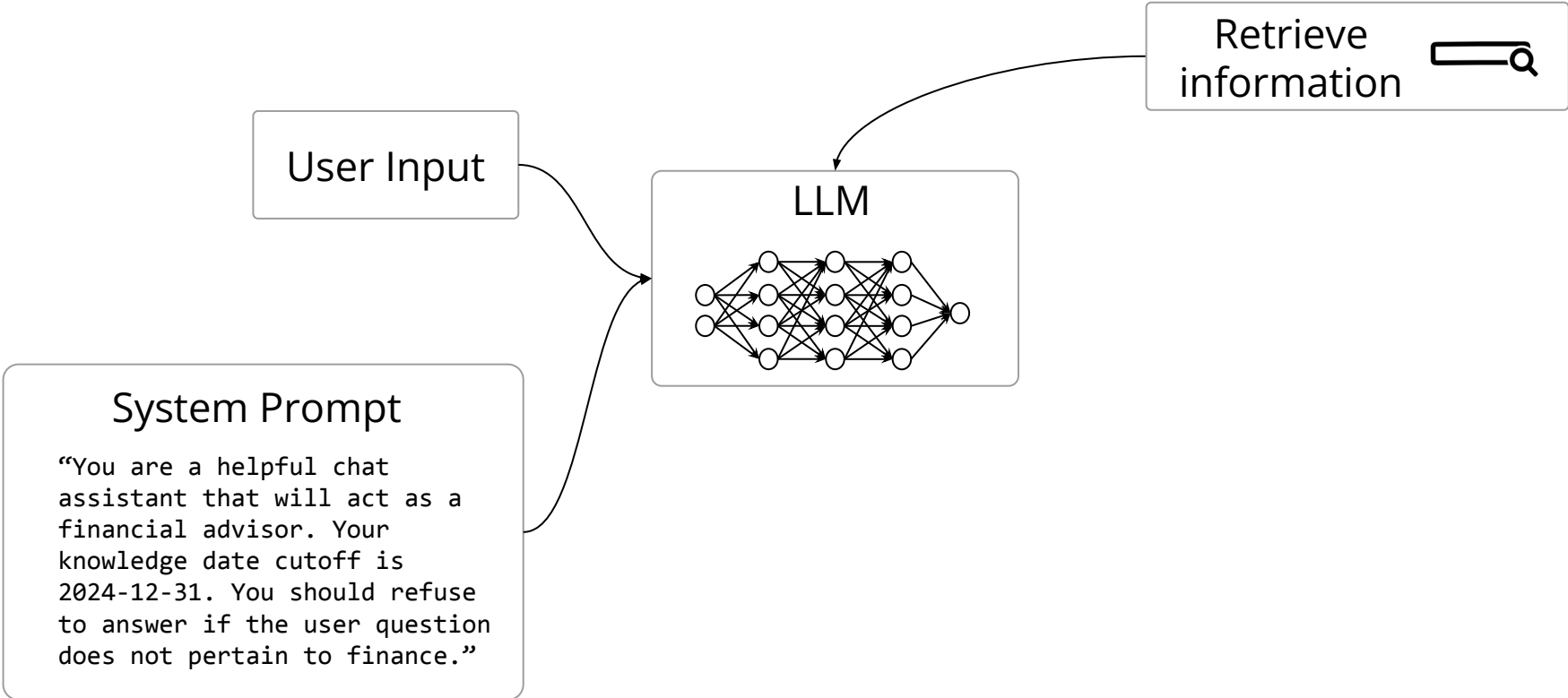
“You are a helpful chat assistant that will act as a financial advisor. Your knowledge date cutoff is 2024-12-31. You should refuse to answer if the user question does not pertain to finance.”



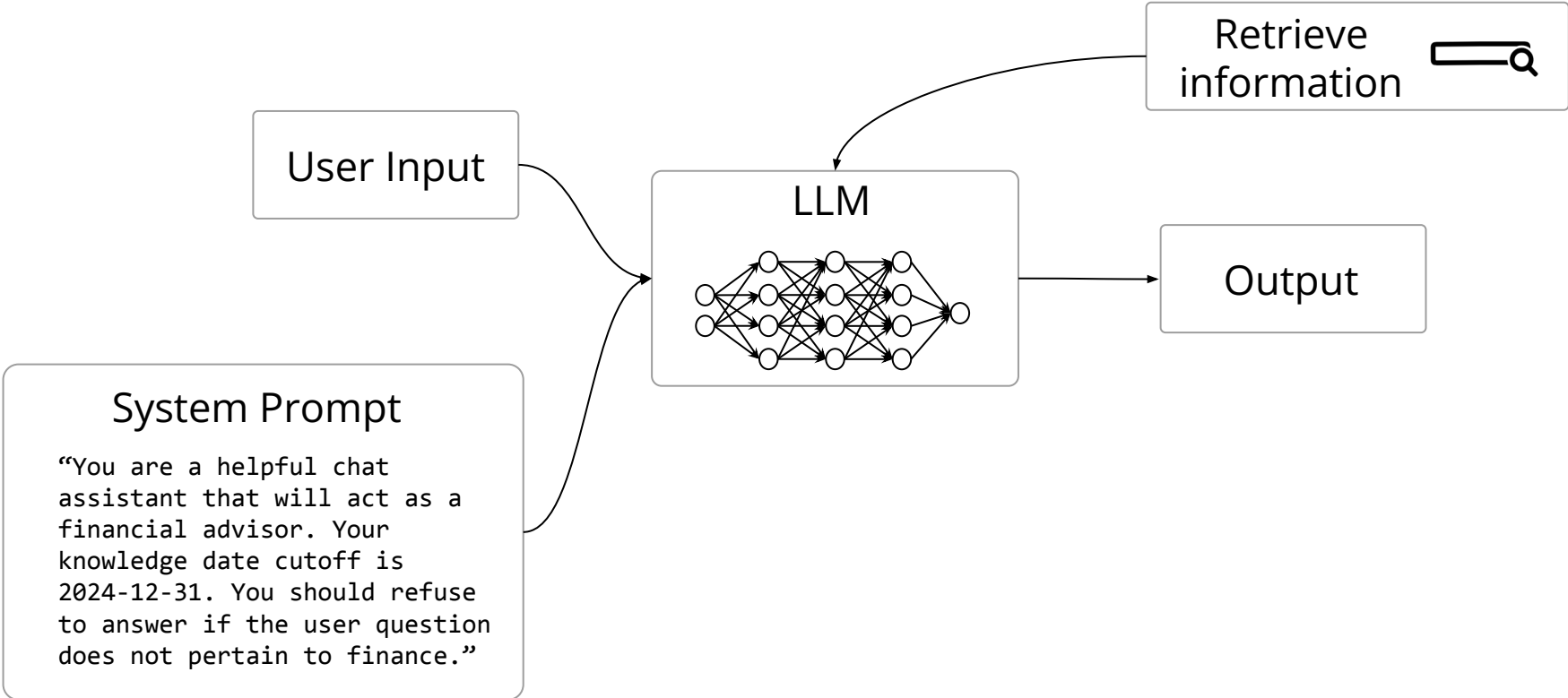
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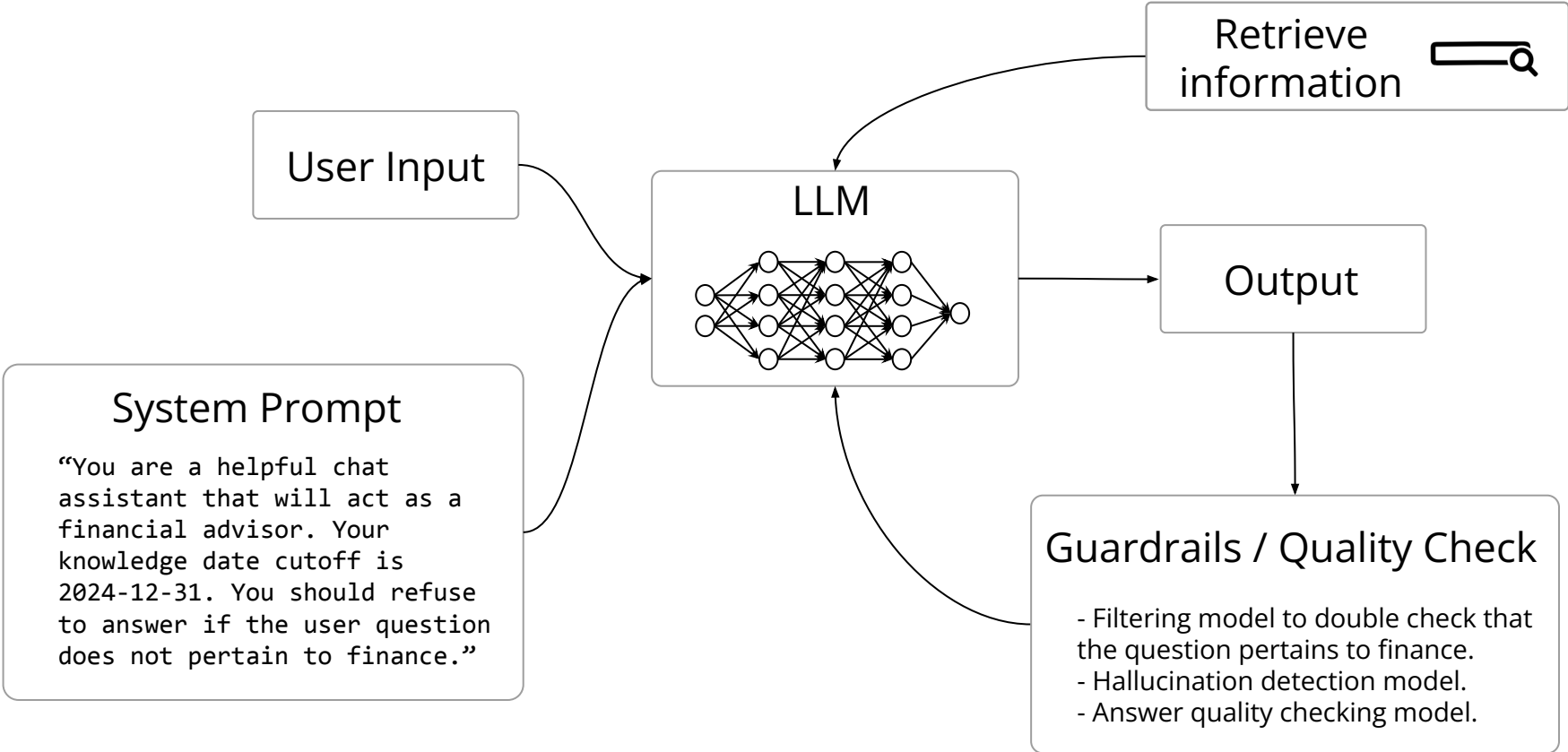
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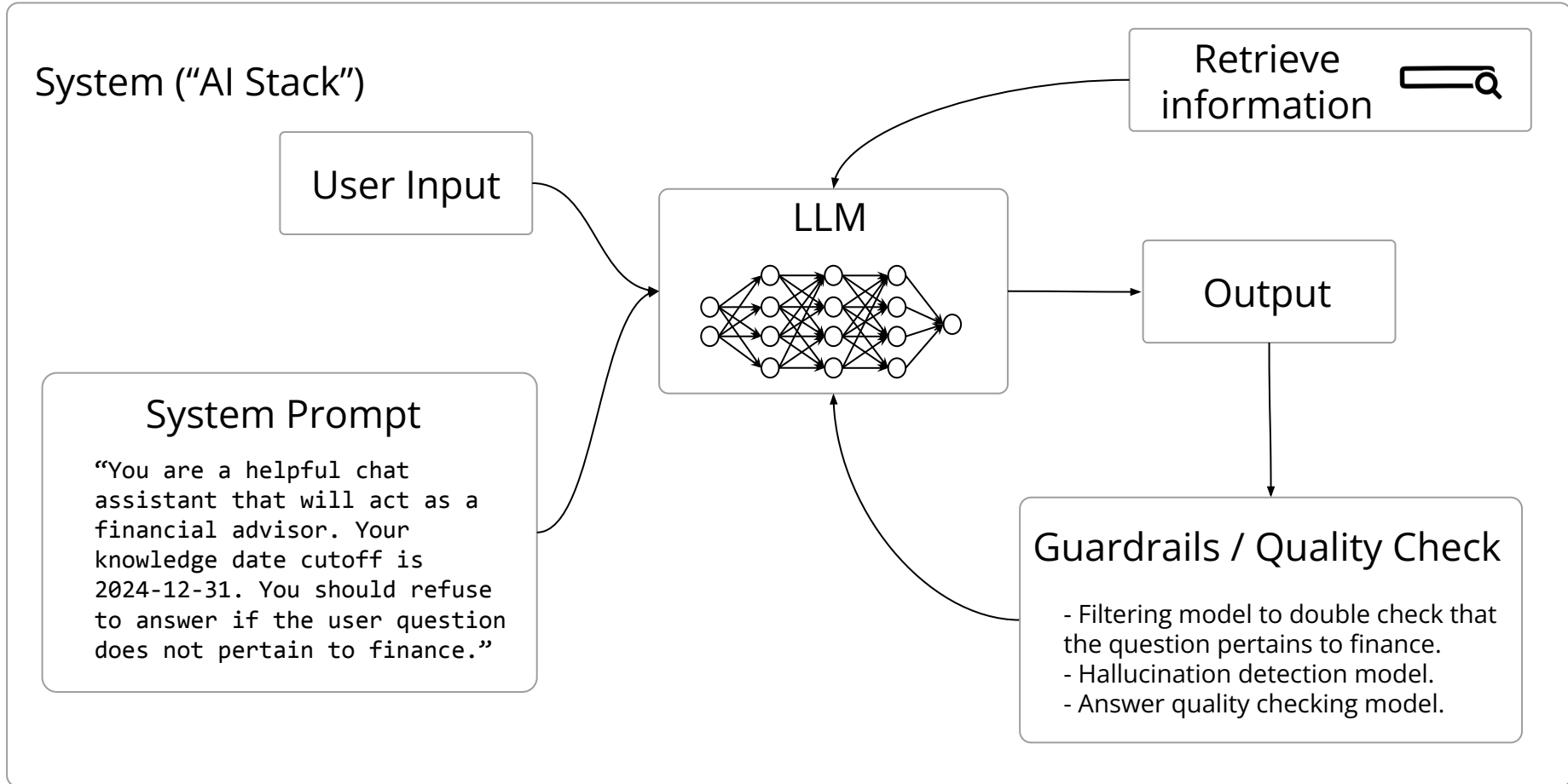
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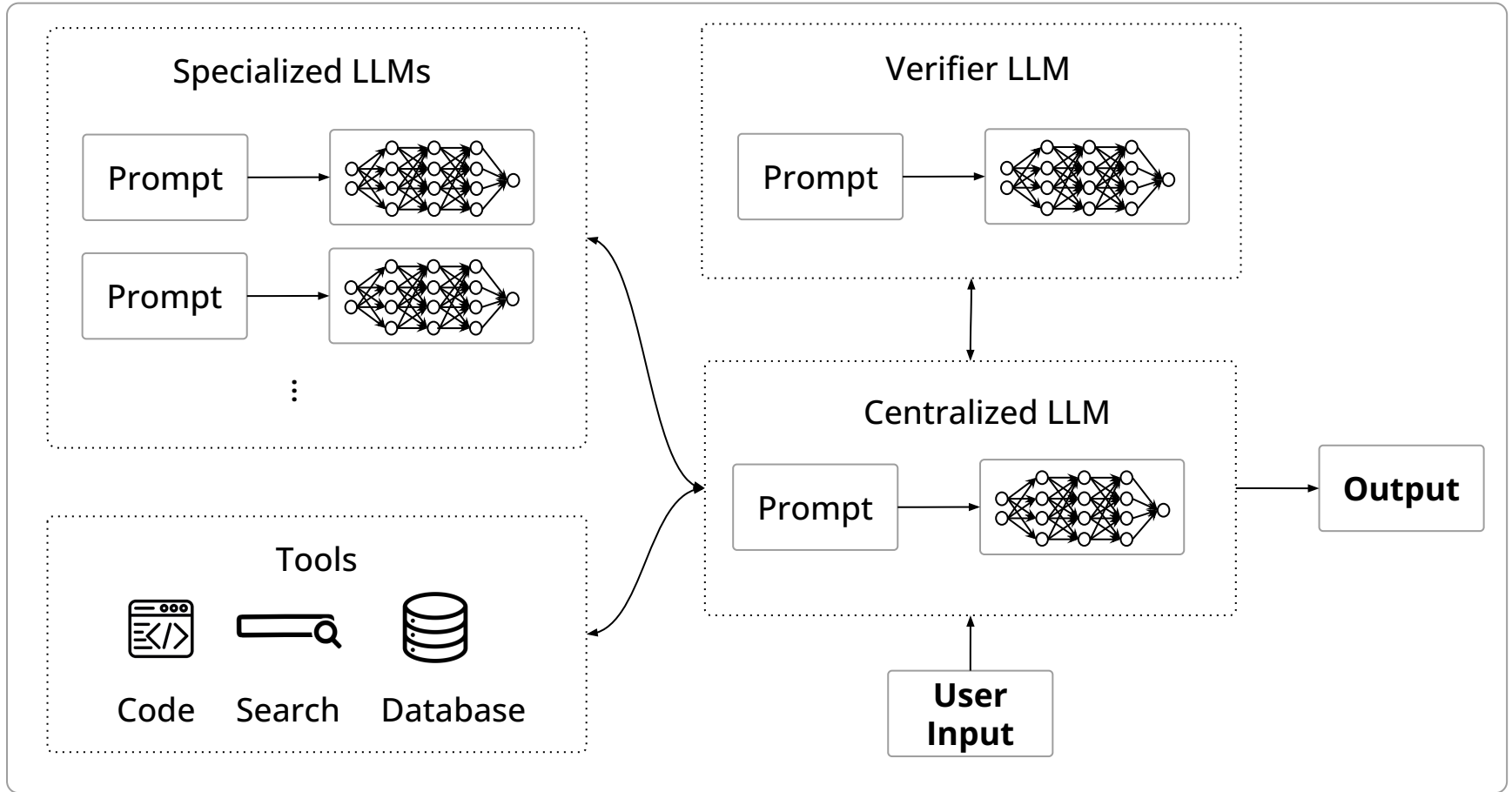
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More complex systems



Part 4 Takeaway

LLMs are developed via two stages: pre-training and post-training.

Pre-training allows LLMs learn broad knowledge. Post-training sharpens its capabilities as assistants/researchers.

Post-training is typically done via reinforcement learning on different types of rewards.

LLMs are used as part of broader AI systems.

Thanks!