EEP 596: LLMs: From Transformers to GPT || Lecture 8

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Logistics

- MP1, Part 2 released today and due two Fridays from now
- Paper Presentation: Please stick to schedule. Notify us if you like a change in date, and we can look into it.

Last Lecture

- Multi-Head Attention

Today's Lecture

- Multi-Head Attention Continued
- Feed Forward NN
- Training Objectives for BERT
- sBERT
- Paper Presentations

Deep Learning References

Deep Learning

Great reference for the theory and fundamentals of deep learning: Book by Goodfellow and Bengio et al Bengio et al

Deep Learning History

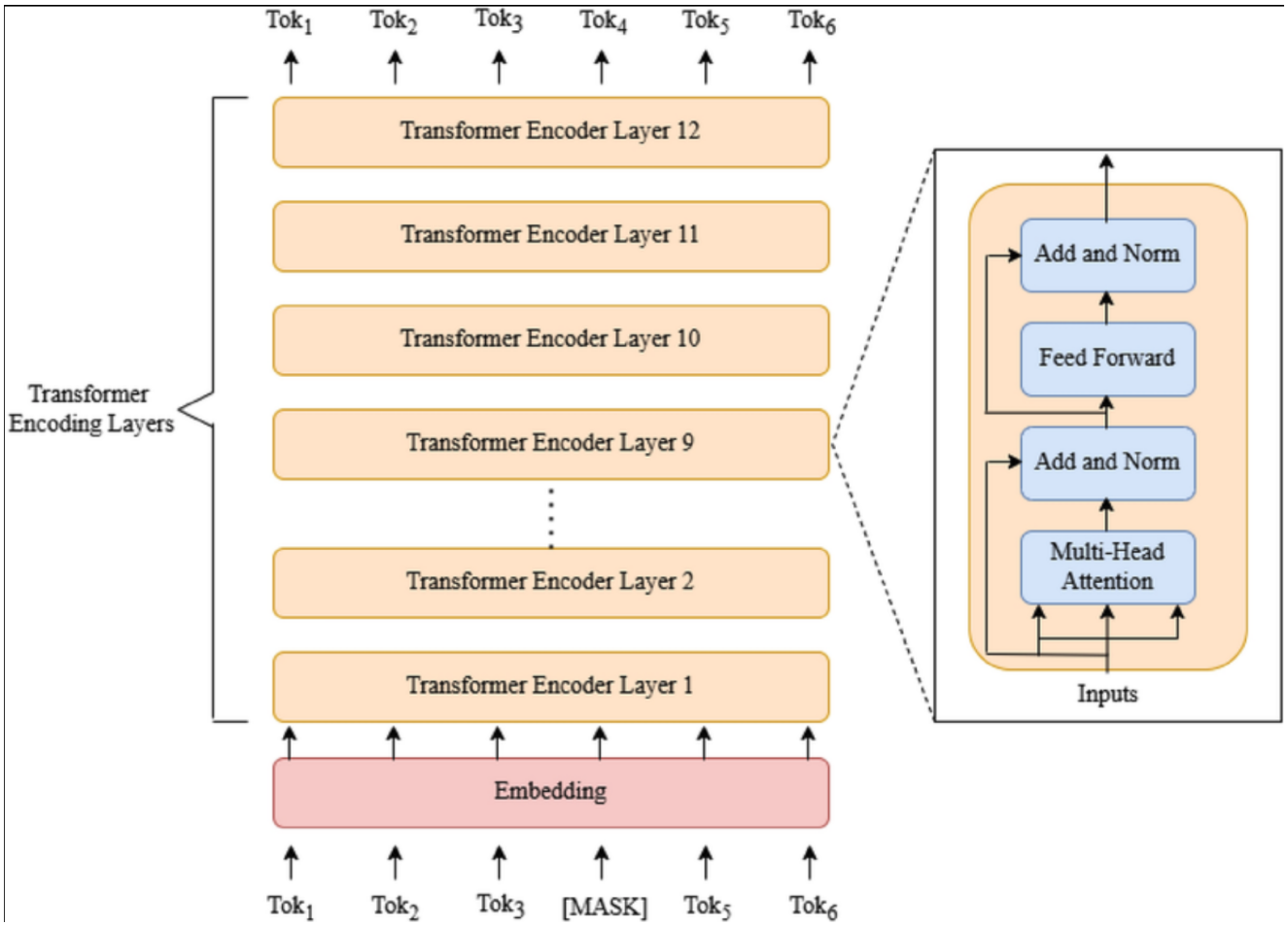
Embeddings

SBERT and its usefulness SBert Details Instacart Search Relevance Instacart Auto-Complete

Attention

Illustration of attention mechanism

BERT Encoding Layers



Transformation through Self-Attention and FFN

Setup (Before Layer 0)

Tokens

```
css

["thinking", "machines"]
```

Embedding size

- **d_model = 768**
- Number of tokens **T = 2**

Transformation through Self-Attention and FFN

1️⃣ Input embeddings (Layer 0 input)

Each token gets:

- **Token embedding**
- **Position embedding**
- **Segment embedding**

They are **summed**:

$$x_i^{(0)} = E_{\text{token}}(i) + E_{\text{position}}(i) + E_{\text{segment}}(i)$$

So we have:

$$X^{(0)} = \begin{bmatrix} x_{\text{thinking}} \\ x_{\text{machines}} \end{bmatrix} \in \mathbb{R}^{2\times 768}$$

This matrix is the **input to Layer 0**.

Transformation through Self-Attention and FFN

2 Self-Attention: Create Q, K, V

BERT uses **multi-head attention**.

- Heads = 12
- Head dimension = $d_k = 768/12 = 64$

For **each head h**, we learn matrices:

$$W_Q^{(h)}, W_K^{(h)}, W_V^{(h)} \in \mathbb{R}^{768\times 64}$$

Compute Q, K, V

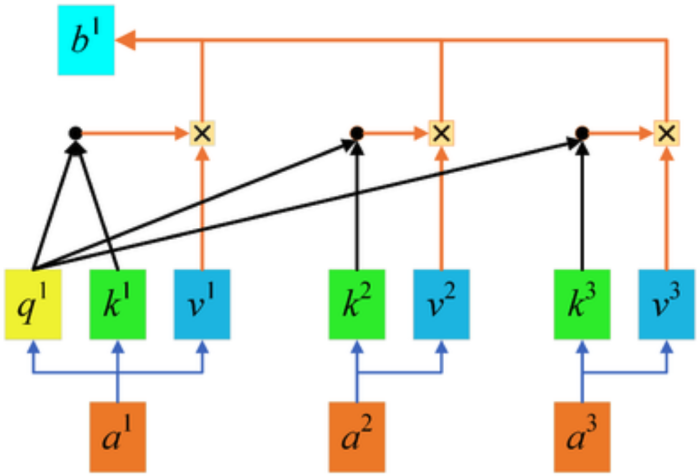
For both tokens:

$$Q = X^{(0)}W_Q \quad K = X^{(0)}W_K \quad V = X^{(0)}W_V$$

Each is:

$$Q, K, V \in \mathbb{R}^{2\times 64}$$

Transformation through Self-Attention and FFN



(a)

$q^i = W^q a^i$ $\quad q^1\ q^2\ q^3 = W^q\ a^1\ a^2\ a^3$, Q

$k^i = W^k a^i$ $\quad k^1\ k^2\ k^3 = W^k\ a^1\ a^2\ a^3$, K

$v^i = W^v a^i$ $\quad v^1\ v^2\ v^3 = W^v\ a^1\ a^2\ a^3$, V

(b)

Transformation through Self-Attention and FFN

3️⃣ Attention scores (who looks at whom)

Compute **scaled dot-product attention**:

$$A = \frac{QK^\top}{\sqrt{d_k}}$$

So:

$$A \in \mathbb{R}^{2\times 2}$$

Example interpretation:

```
ini

A =
[ thinking→thinking   thinking→machines
  machines→thinking   machines→machines ]
```

Each value = *similarity of queries to keys*.

Transformation through Self-Attention and FFN

4 Softmax (turn scores into weights)

Row-wise softmax:

$$\alpha_{ij} = \frac{e^{A_{ij}}}{\sum_j e^{A_{ij}}}$$

Now each row sums to 1.

This answers:

> "How much should **thinking** attend to itself vs **machines**?"

Transformation through Self-Attention and FFN

5 Weighted sum of values

$$Z = \alpha V$$

Result:

$$Z \in \mathbb{R}^{2\times 64}$$

Meaning:

- "thinking" becomes a **contextual blend** of thinking + machines
- same for "machines"

Transformation through Self-Attention and FFN

6 Concatenate heads + output projection

After doing this for **all 12 heads**:

$$Z_{\text{concat}} \in \mathbb{R}^{2\times 768}$$

Final projection:

$$Z_{\text{attn}} = Z_{\text{concat}} W_O \quad W_O \in \mathbb{R}^{768\times 768}$$

Transformation through Self-Attention and FFN

7️⃣ Residual connection + LayerNorm

$$\tilde{X} = \text{LayerNorm}(X^{(0)} + Z_{\text{attn}})$$

This stabilizes training and preserves original info.

🔶 Feed-Forward Network (FFN)

Now each token is processed **independently** (no cross-token mixing here).

Transformation through Self-Attention and FFN

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8️⃣ First linear layer (expansion)

$$H = \tilde{X}W_1 + b_1$$

Where:

- $W_1 \in \mathbb{R}^{768\times3072}$

Result:

$$H \in \mathbb{R}^{2\times3072}$$

9️⃣ GELU activation

$$\mathrm{GELU}(x) = x \cdot \Phi(x)$$

This introduces **nonlinearity** (soft gating).

Transformation through Self-Attention and FFN

🔟 Second linear layer (compression)

$$F = \text{GELU}(H)W_2 + b_2$$

Where:

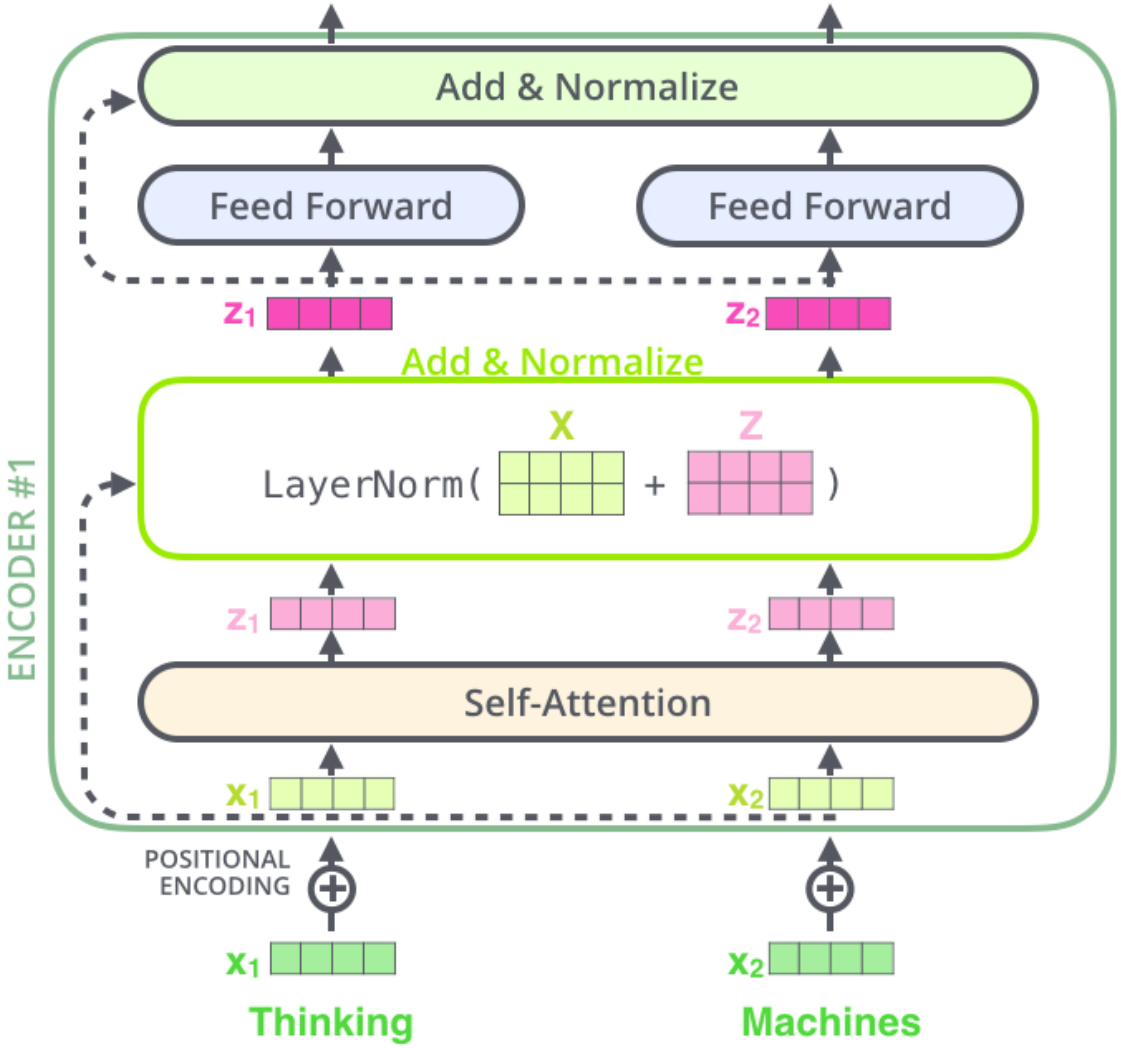
- $W_2 \in \mathbb{R}^{3072 \times 768}$

1️⃣1️⃣ Residual + LayerNorm (end of layer)

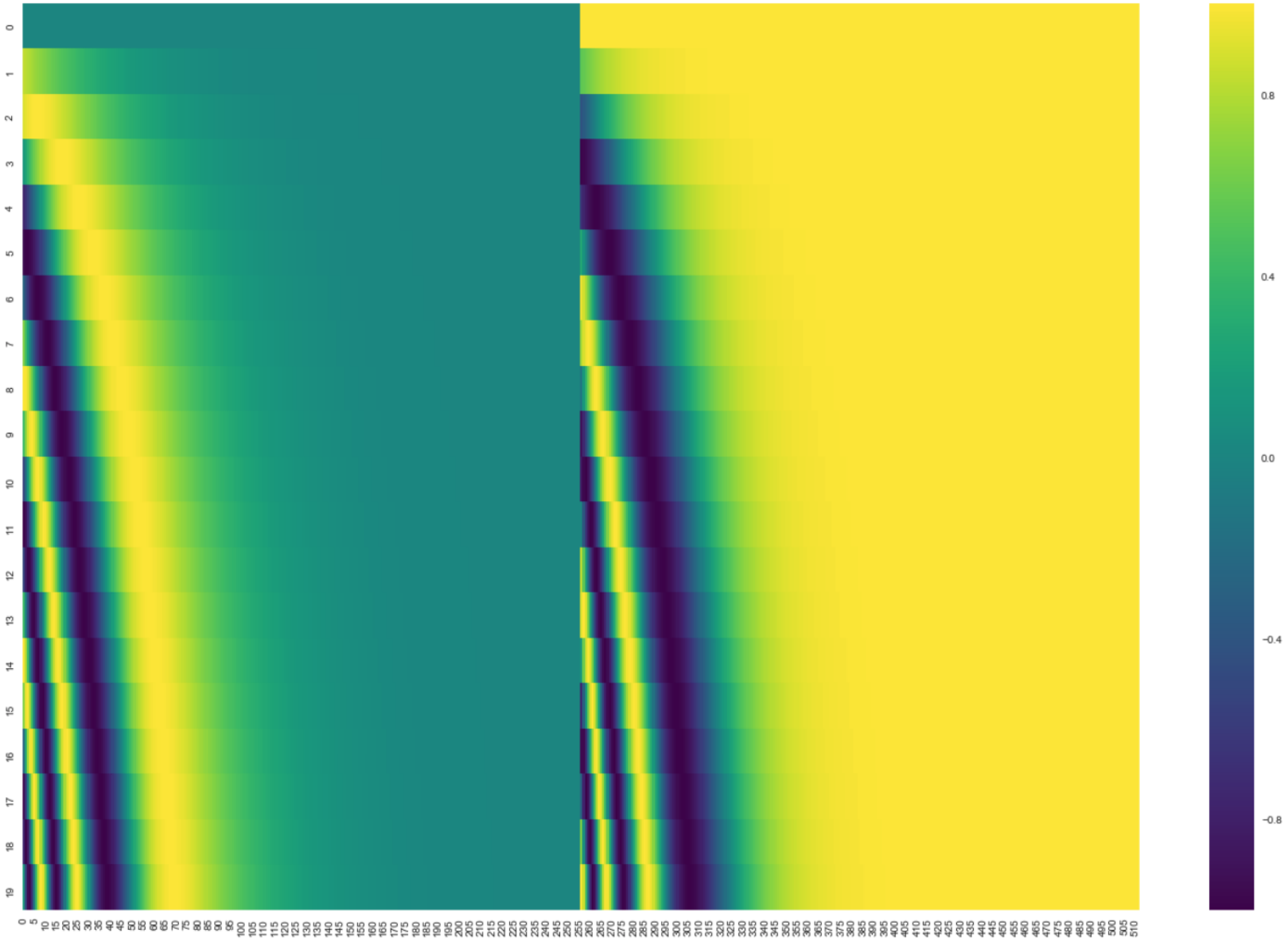
$$X^{(1)} = \text{LayerNorm}(\tilde{X} + F)$$

This is the **output of Layer 1**.

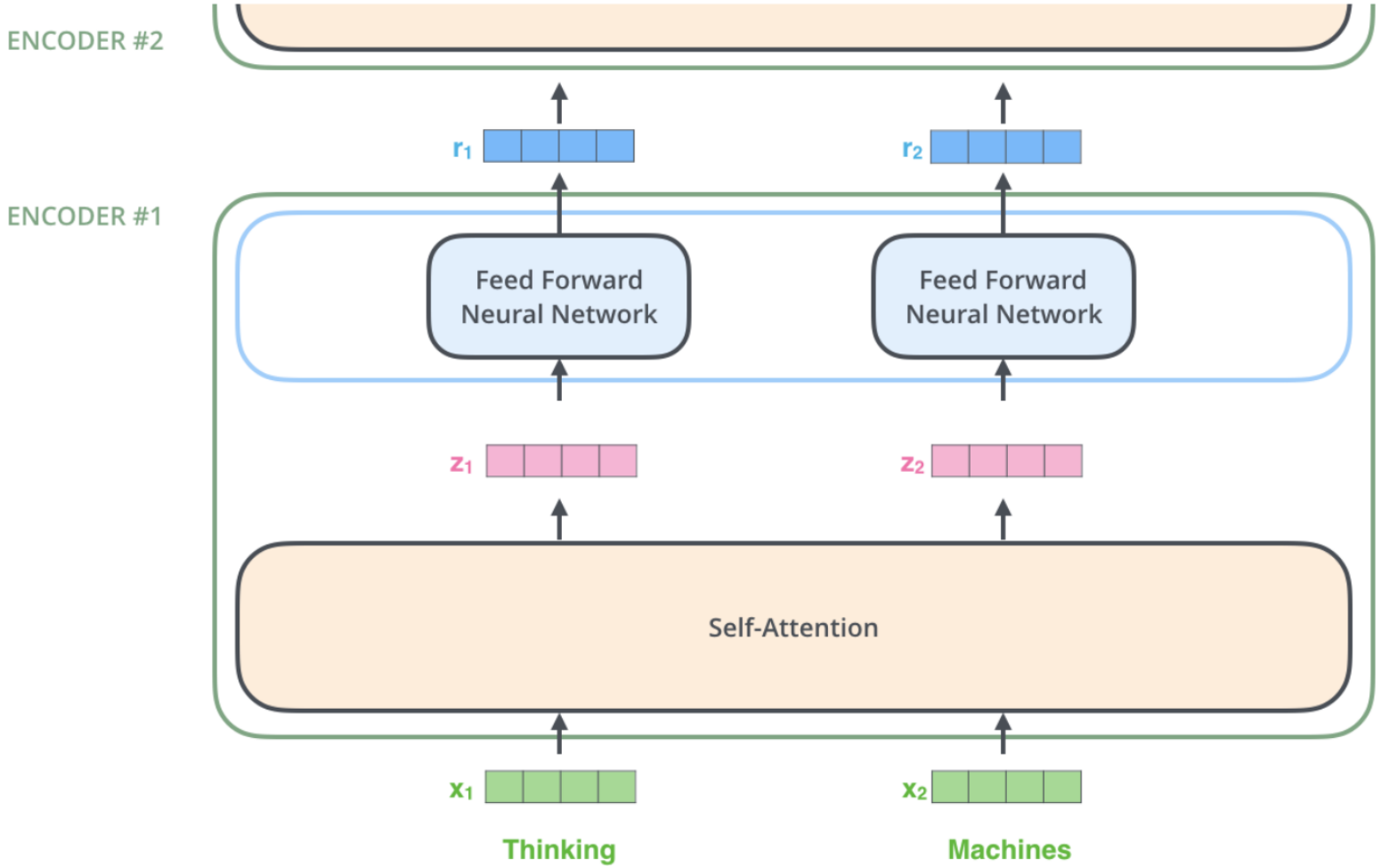
Parsing Encoder: Multi-Head Attention and FFN



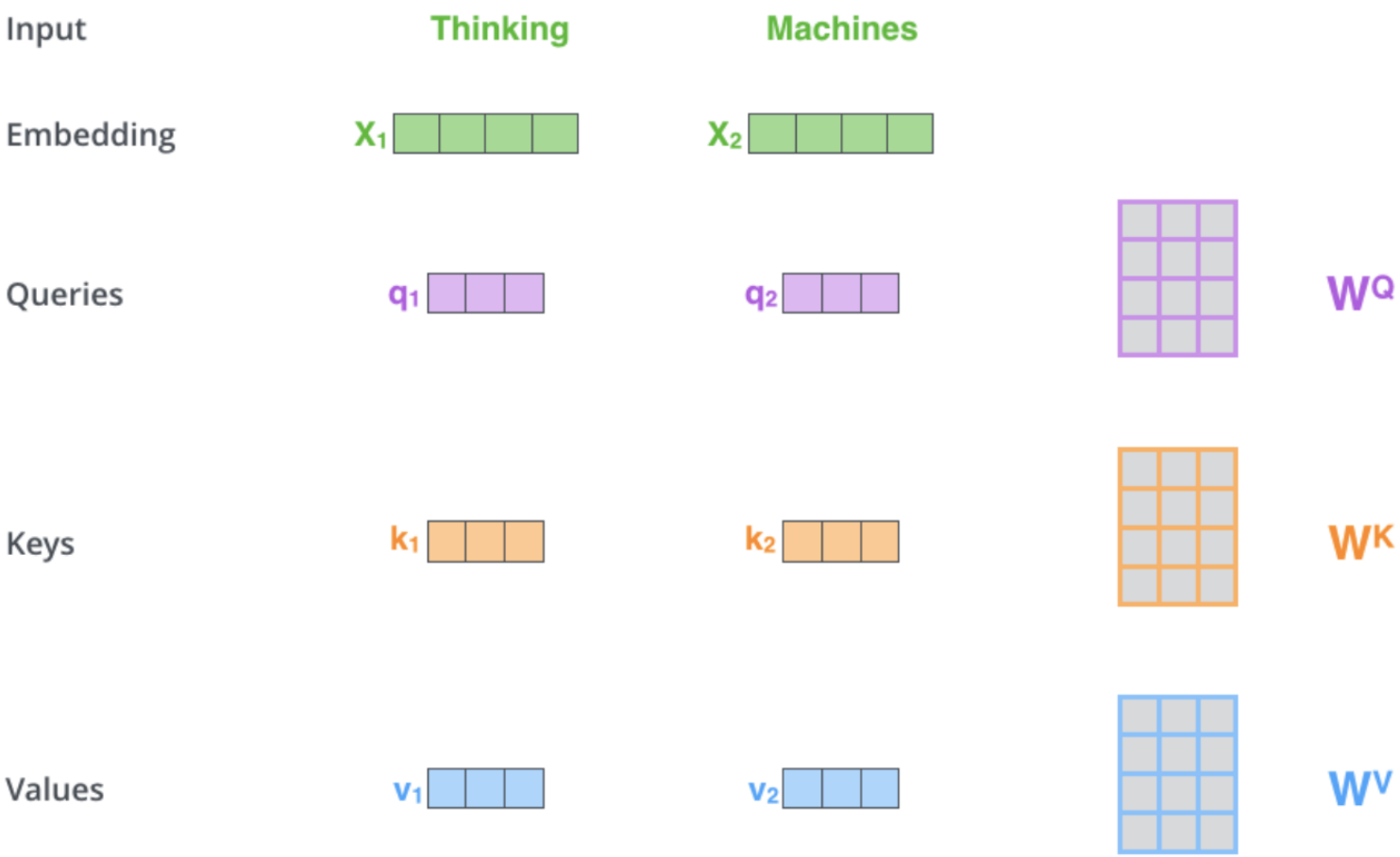
Positional Encoding



Parsing Encoder: Multi-Head Attention and FFN



Parsing Encoder: Single Head Attention



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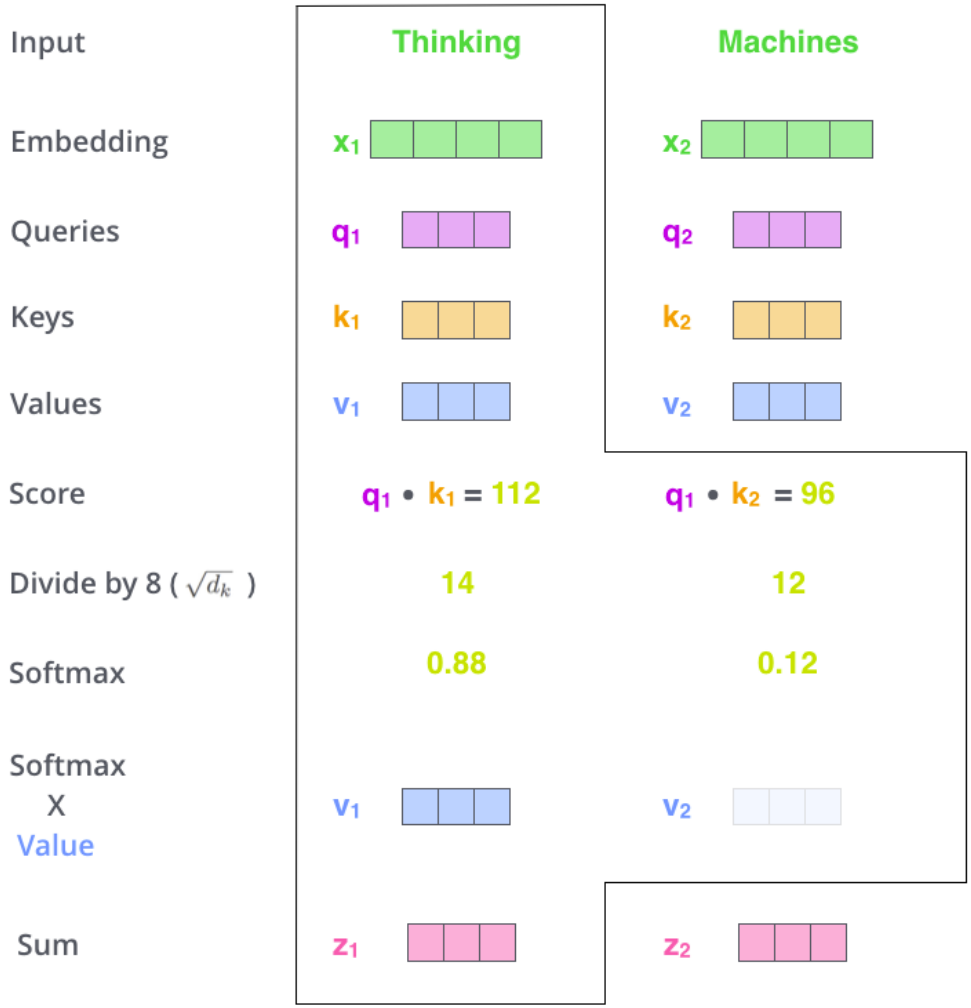

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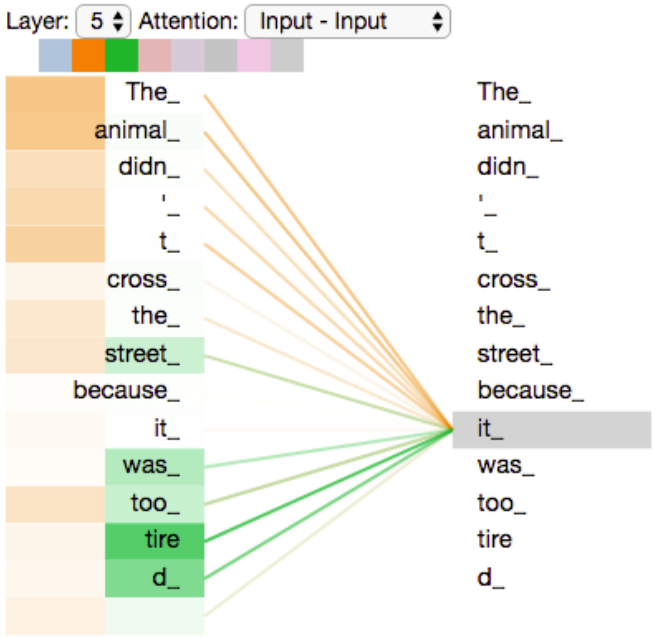
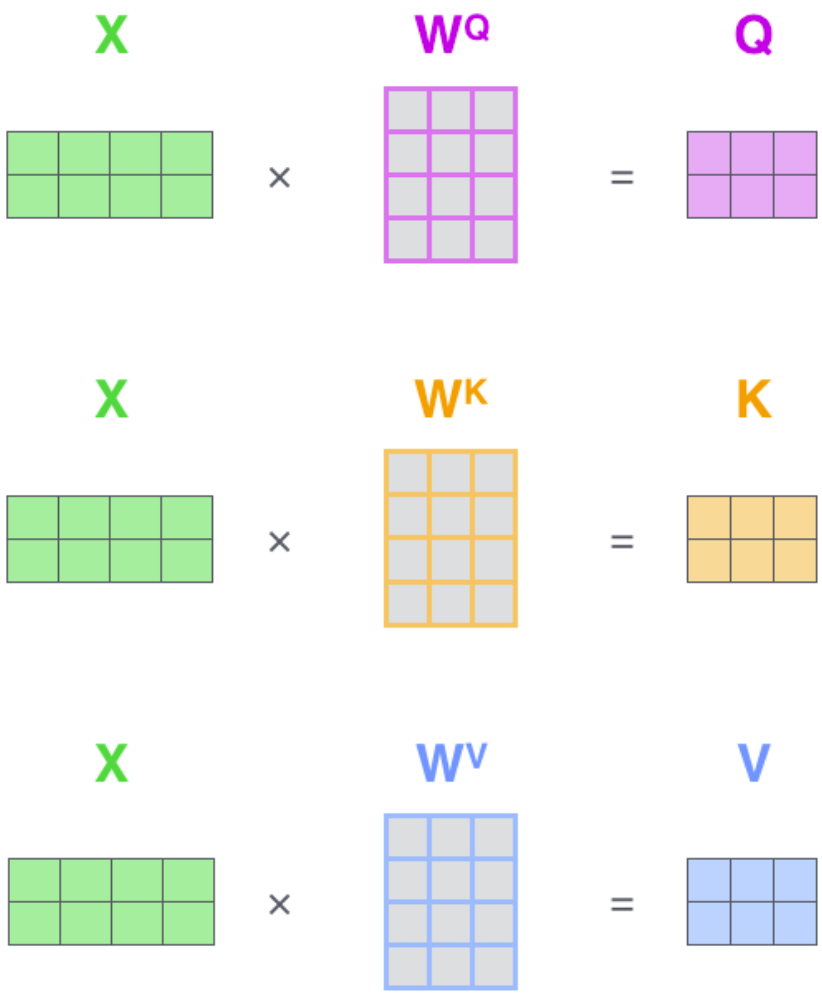


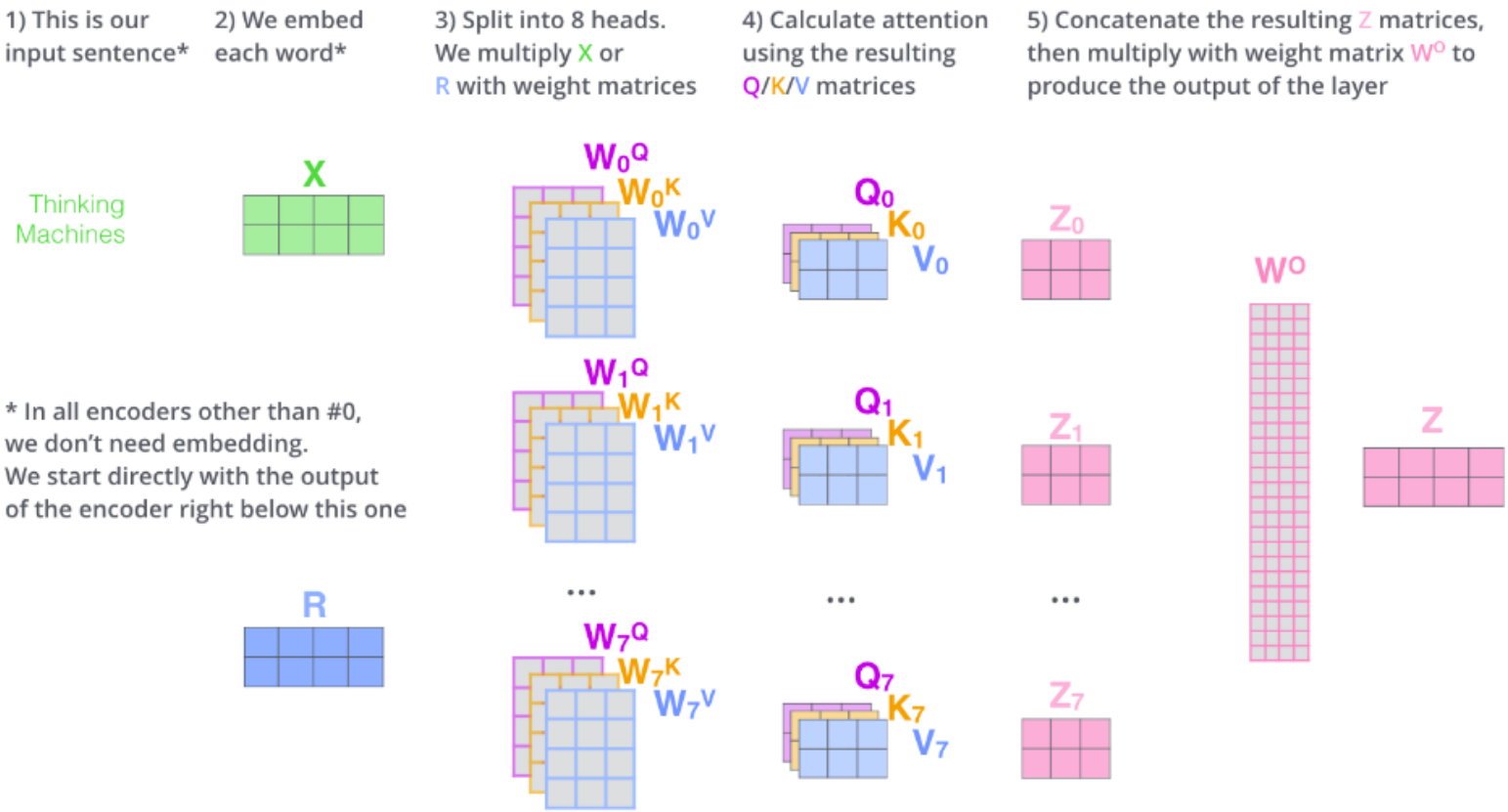
As we encode the word "it", one attention head is focusing most on "the animal", while another is focusing on "tired" -- in a sense, the model's representation of the word "it" bakes in some of the representation of both "animal" and "tired".

Parsing Encoder: Single Head Attention

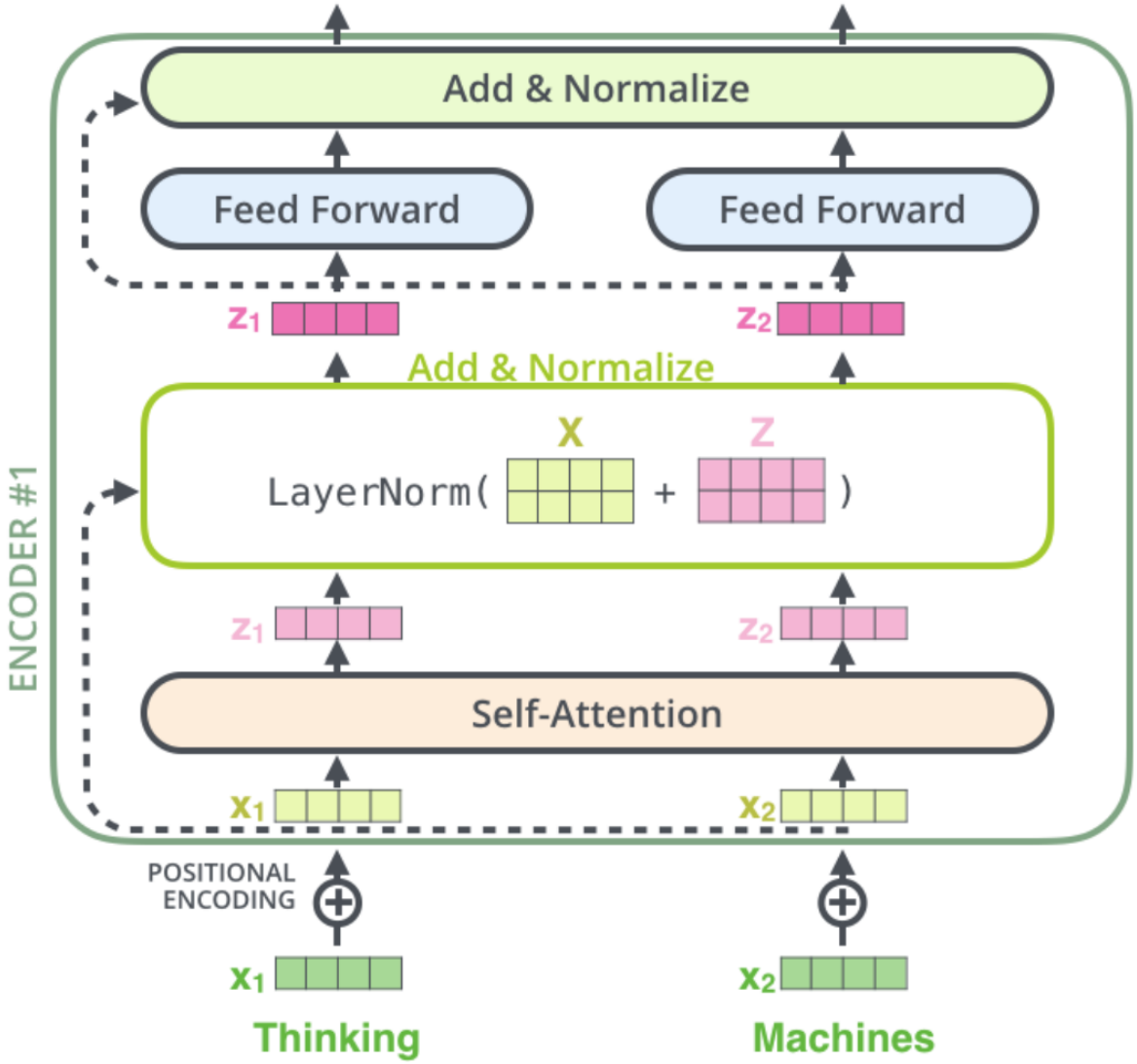


Every row in the X matrix corresponds to a word in the input sentence. We again see the difference in size of the embedding vector (512, or 4 boxes in the figure), and the q/k/v vectors (64, or 3 boxes in the figure)

Parsing Encoder: Multi-Head Attention and FFN



Layer Normalization



Self-Attention vs FFN

- Self-Attention: Communication between tokens, better understanding of context for each token
- FFN: Deeper representation of each token. Each token reasons internally, deeper thinking.
- What if there was no self-attention: Reduces to a Deep Neural Network or Recurrent Neural Network
- What if there was no FFN: The deeper learning and deeper representations would be missed

ICE #1: Self-attention Exercise

Let's go through a self-attention python calculation exercise to understand it better. Let $x = [[1, 2, 3, -1], [3, -4, -7, 5]]$ be the input token embeddings. In the first layer of the encoder of the transformer, the weight matrices are given by $W^Q = [[-1, 2, 0], [2, 3, -5], [1, 0, 0], [-3, 1, 2]]$,
$W^K = [[1, 2, 3], [2, 4, 3], [3, 0, 3], [-1, 5, 2]]$,
$W^V = [[-1, -2, 3], [2, -4, 0], [0, 0, 1], [1, 0, -7]]$. Compute the soft-max similar to what we did in the previous walk-through. You can use python matrix multiplication (e.g. numpy) to arrive at the solution. Question is which token (token 1 or token 2) does token 2 place more attention on and what is the attention probability?

BERT pre-training

Two Tasks

1. **Masked LM Model:** Mask a word in the middle of a sentence and have BERT predict the masked word
2. **Next-sentence prediction:** Predict the next sentence - Use both positive and negative labels. How are these generated?

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ICE: Supervised or Un-supervised?

1. Are the above two tasks supervised or un-supervised?

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Data set!

English Wikipedia and book corpus documents!

Loss Function for Masked Language Model (MLM)

Loss Function for MLM mimicks which type of classic ML model?

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Cross-Entropy

$$L(p, \hat{p}) = -\sum_i [p_i \log(\hat{p}_i) + (1 - p_i) \log(1 - \hat{p}_i)]$$

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ICE: What is the loss function for Binary Classification?

Sentence BERT a.k.a sBERT

Uses Siamese Twins architecture

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Advantages of sBERT

More optimized for Sentence Similarity Search.

Sentence BERT - Siamese BERT architecture

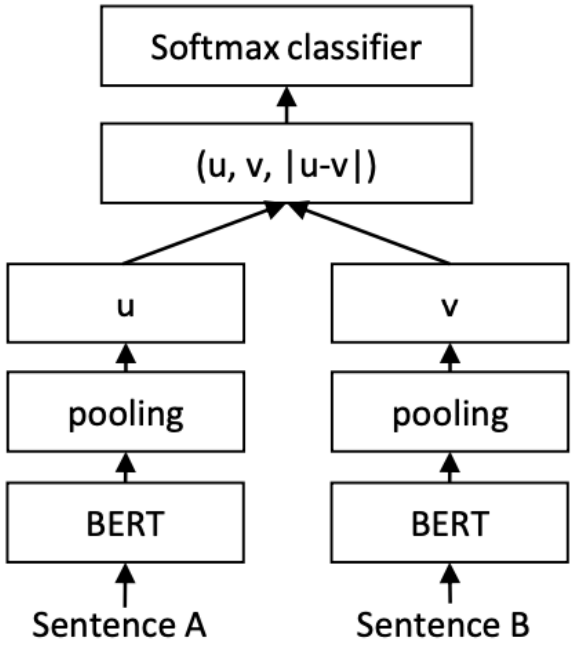

Figure 1: SBERT architecture with classification objective function, e.g., for fine-tuning on SNLI dataset. The two BERT networks have tied weights (siamese network structure).

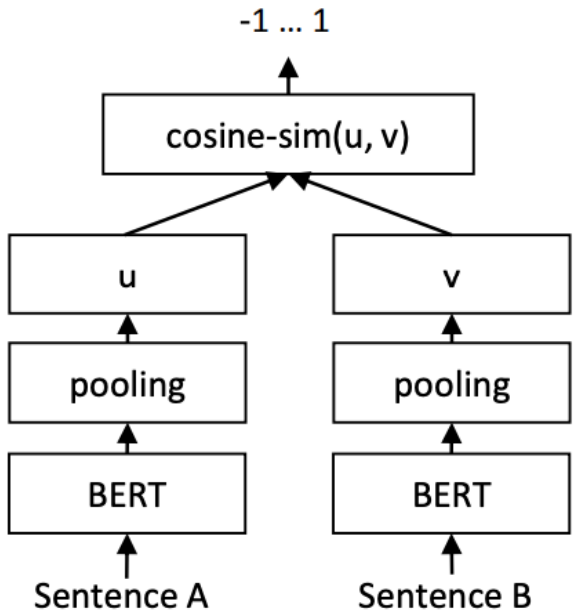

Figure 2: SBERT architecture at inference, for example, to compute similarity scores. This architecture is also used with the regression objective function.

Pooling Strategy for SBERT

	NLI	STSb
Pooling Strategy		
MEAN	**80.78**	**87.44**
MAX	79.07	69.92
CLS	79.80	86.62
Concatenation		
(u, v)	66.04	-
$(\|u - v\|)$	69.78	-
$(u * v)$	70.54	-
$(\|u - v\|, u * v)$	78.37	-
$(u, v, u * v)$	77.44	-
$(u, v, \|u - v\|)$	**80.78**	-
$(u, v, \|u - v\|, u * v)$	80.44	-

Table 6: SBERT trained on NLI data with the classification objective function, on the STS benchmark (STSb) with the regression objective function. Configurations are evaluated on the development set of the STSb using cosine-similarity and Spearman's rank correlation. For the concatenation methods, we only report scores with MEAN pooling strategy.

Sentence BERT Cosine Similarity Results

Model	STS12	STS13	STS14	STS15	STS16	STSb	SICK-R	Avg.
Avg. GloVe embeddings	55.14	70.66	59.73	68.25	63.66	58.02	53.76	61.32
Avg. BERT embeddings	38.78	57.98	57.98	63.15	61.06	46.35	58.40	54.81
BERT CLS-vector	20.16	30.01	20.09	36.88	38.08	16.50	42.63	29.19
InferSent - Glove	52.86	66.75	62.15	72.77	66.87	68.03	65.65	65.01
Universal Sentence Encoder	64.49	67.80	64.61	76.83	73.18	74.92	**76.69**	71.22
SBERT-NLI-base	70.97	76.53	73.19	79.09	74.30	77.03	72.91	74.89
SBERT-NLI-large	72.27	**78.46**	**74.90**	80.99	76.25	**79.23**	73.75	76.55
SRoBERTa-NLI-base	71.54	72.49	70.80	78.74	73.69	77.77	74.46	74.21
SRoBERTa-NLI-large	**74.53**	77.00	73.18	**81.85**	**76.82**	79.10	74.29	**76.68**

Table 1: Spearman rank correlation ρ between the cosine similarity of sentence representations and the gold labels for various Textual Similarity (STS) tasks. Performance is reported by convention as $\rho \times 100$. STS12-STS16: SemEval 2012-2016, STSb: STSbenchmark, SICK-R: SICK relatedness dataset.

SentEval DataSets

- **MR**: Sentiment prediction for movie reviews snippets on a five start scale (Pang and Lee, 2005).
- **CR**: Sentiment prediction of customer product reviews (Hu and Liu, 2004).
- **SUBJ**: Subjectivity prediction of sentences from movie reviews and plot summaries (Pang and Lee, 2004).
- **MPQA**: Phrase level opinion polarity classification from newswire (Wiebe et al., 2005).
- **SST**: Stanford Sentiment Treebank with binary labels (Socher et al., 2013).
- **TREC**: Fine grained question-type classification from TREC (Li and Roth, 2002).
- **MRPC**: Microsoft Research Paraphrase Corpus from parallel news sources (Dolan et al., 2004).

Sentence BERT on SentEval Results

Model	MR	CR	SUBJ	MPQA	SST	TREC	MRPC	Avg.
Avg. GloVe embeddings	77.25	78.30	91.17	87.85	80.18	83.0	72.87	81.52
Avg. fast-text embeddings	77.96	79.23	91.68	87.81	82.15	83.6	74.49	82.42
Avg. BERT embeddings	78.66	86.25	94.37	88.66	84.40	92.8	69.45	84.94
BERT CLS-vector	78.68	84.85	94.21	88.23	84.13	91.4	71.13	84.66
InferSent - GloVe	81.57	86.54	92.50	**90.38**	84.18	88.2	75.77	85.59
Universal Sentence Encoder	80.09	85.19	93.98	86.70	86.38	**93.2**	70.14	85.10
SBERT-NLI-base	83.64	89.43	94.39	89.86	88.96	89.6	**76.00**	87.41
SBERT-NLI-large	**84.88**	**90.07**	**94.52**	90.33	**90.66**	87.4	75.94	**87.69**

Table 5: Evaluation of SBERT sentence embeddings using the SentEval toolkit. SentEval evaluates sentence embeddings on different sentence classification tasks by training a logistic regression classifier using the sentence embeddings as features. Scores are based on a 10-fold cross-validation.

ICE #2

Let's say we want to automatically convert a **Natural Language Query** to a **SQL** query. E.g. "Which quarter in the past 5 years had the most amount of sales for fashion products" to "SELECT ... FROM ... WHERE ..." What kind of deep learning architecture would support this problem?

1. SBERT
2. LSTM to LSTM sequence model
3. GPT-2
4. Feed Forward Neural Network

Fine-Tuning Transformers for down-stream tasks

A methodology for fine-tuning transformers for classification tasks

1. **Pick Base pre-trained Architecture:** Pick a base pre-trained architecture as a starting point for your fine-tuning. Example: `bert-base-uncased` is one such pre-trained model that can be loaded through `Hugging Face Transformers Library`

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2. **Extract output from pre-training:** How do you want to use the output from pre-training going into *fine-tuning*? a) Extract embedding from the first token, `CLS` b) Average embeddings of all tokens as a starting point (mean pooling).

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3. **Add fine-tuning layers:** Add fine-tuning layers on top of the pre-trained layers. Example, starting with the pooled embeddings, construct one or more dense layers (`Feed-Forward NN style`) to extract finer representations of the input. Add the output layer and its activation (typically softmax for classification tasks).

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4. **Set training schedule, hyper-parameters, etc:** Set up optimizer (e.g. ADAM), hyper-parameters, training schedule, etc for training.

ICE #3

BERT Embeddings and Emotion Detection

Let's say you want to do emotion detection by fine-tuning BERT (Encoding Transformer) on a data set. One of the outputs of the *BERT pre-trained model* for a given input is the *last-hidden-state*. This includes an embedding for every token that was passed into BERT.
Let's say you are going to start with the last hidden layer and use that as input for your *fine-tuned* model. This ICE is about the dimensionality of the inputs and outputs. Let's say you have sentences of the kind: "I am looking forward to today! It's going to be a big day" This sentence conveys excitement. There are 13 words in this input and using *word-piece tokenization*, you arrive at 20 sub-tokens as input into the BERT model. The last hidden layer includes an embedding for every single token. Let's say the embedding dimension for a token is 768.

ICE #3 continued

BERT Embeddings and Emotion Detection

There are 13 words in this input and using *word-piece tokenization*, you arrive at 20 sub-tokens as input into the BERT model. The last hidden layer includes an embedding for every single token. Let's say the embedding dimension for a token is 768. For the purpose of emotion detection - You can either use the *CLS* token (Start token) embedding (also called the pooled embedding) or you can take the average of the embeddings of the tokens in the last hidden layer of BERT. a) What's the dimension of the pooled BERT embedding of this particular input example b) What's the dimension of the CLS/Start token embedding in this example? c) what's the total dimension of the last hidden layer?

1. 768, 15630 and 768
2. 768, 768 and 768
3. 15360, 768 and 15630
4. 768, 768 and 15360

ICE #4

Why does pooling of the output need to be done for sequence classification (e.g. emotion detection)?

1. Reduces the dimensionality
2. Averages context from all the tokens
3. Computational concerns for training the fine-tuned model
4. All of the above

Application of SBERT Embeddings to Instacart Recommendations

Instacart Recommendations

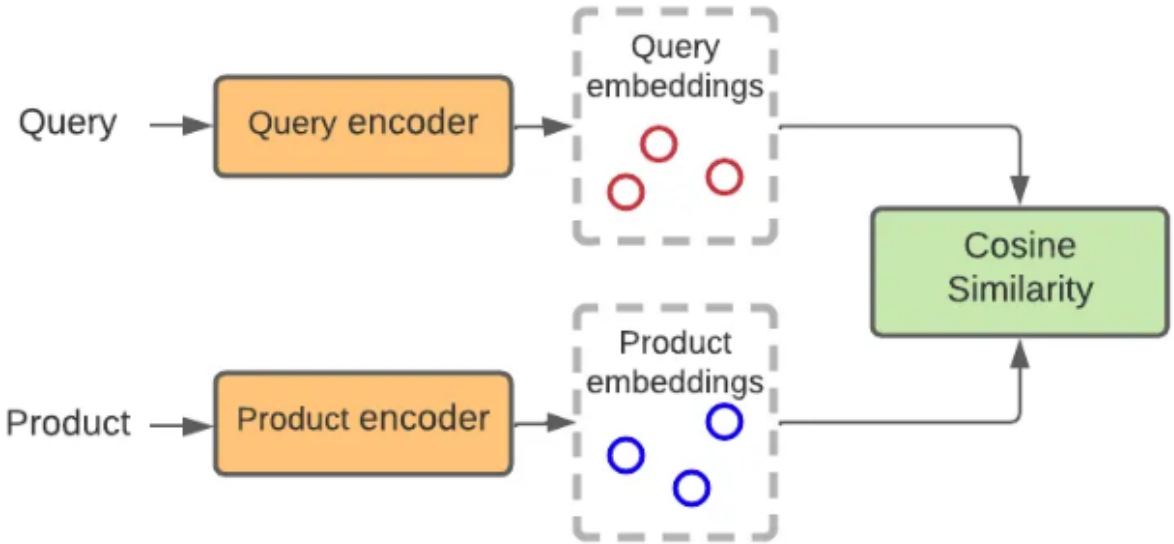
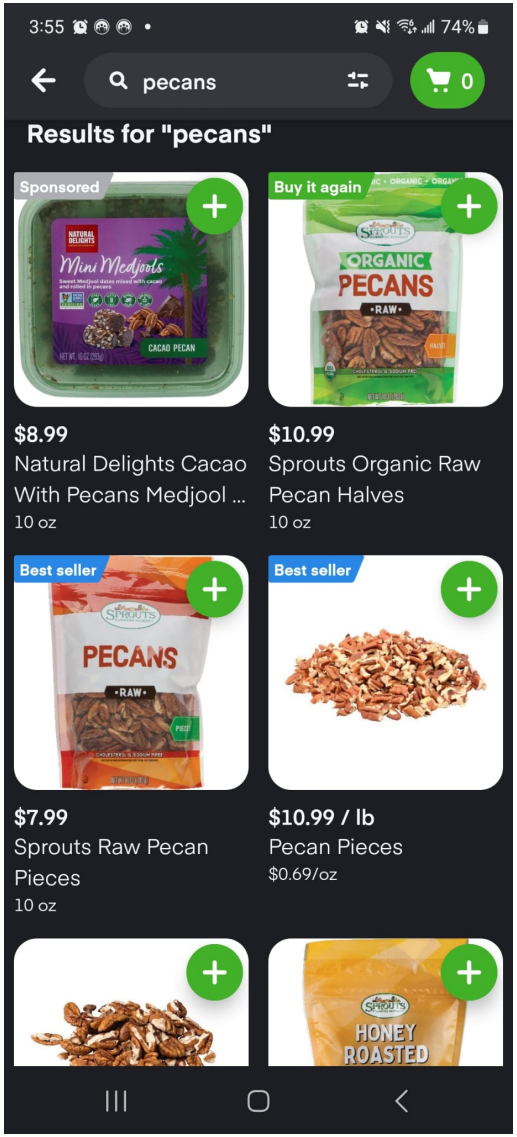


Figure 1. Conceptual diagram of a two-tower model

Positive Examples



High-quality Positive Examples

Converted Products for Search Query “Orange”
Navel Oranges
Clementines
Mandarins
…
Bananas
…
Strawberries

Negative Examples

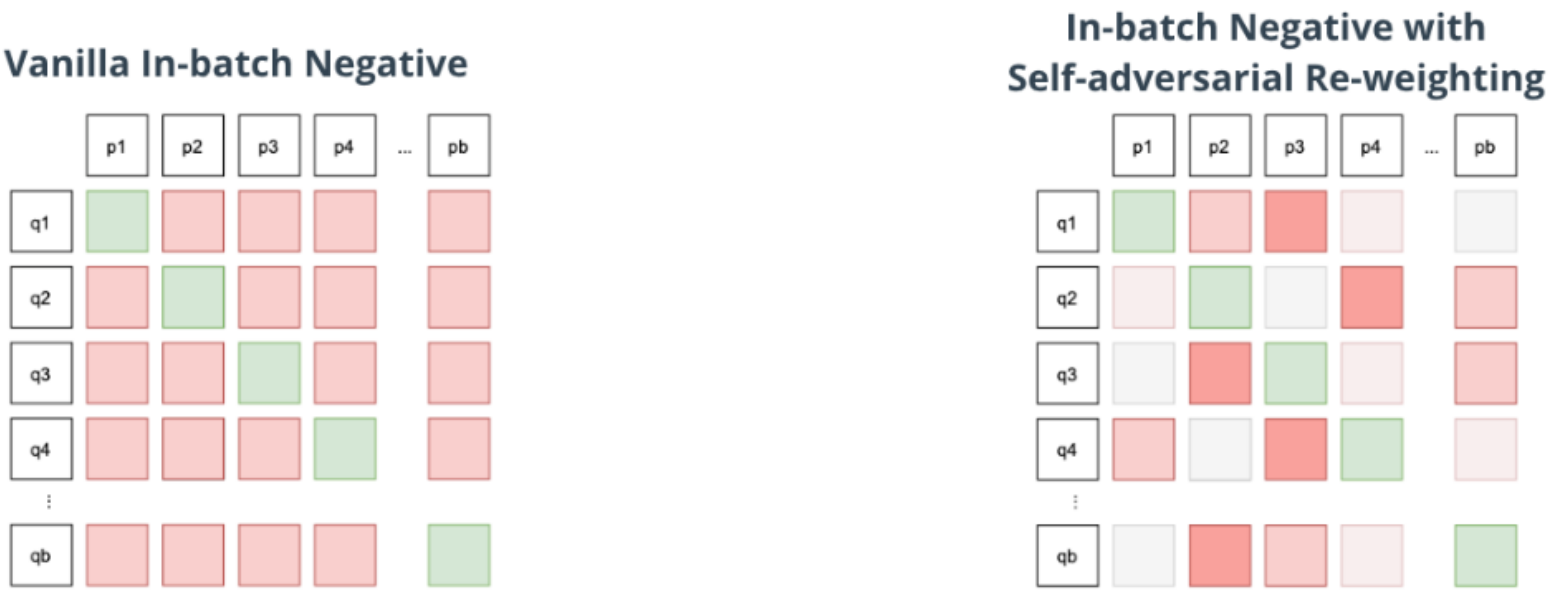


Figure 3. (Left) In the vanilla implementation of in-batch negative, all off-diagonal negative samples are given the same weight. (Right) In our implementation with self-adversarial re-weighting, harder examples are given more weight (darker color), making the task more challenging for the model.

Model Training Architecture

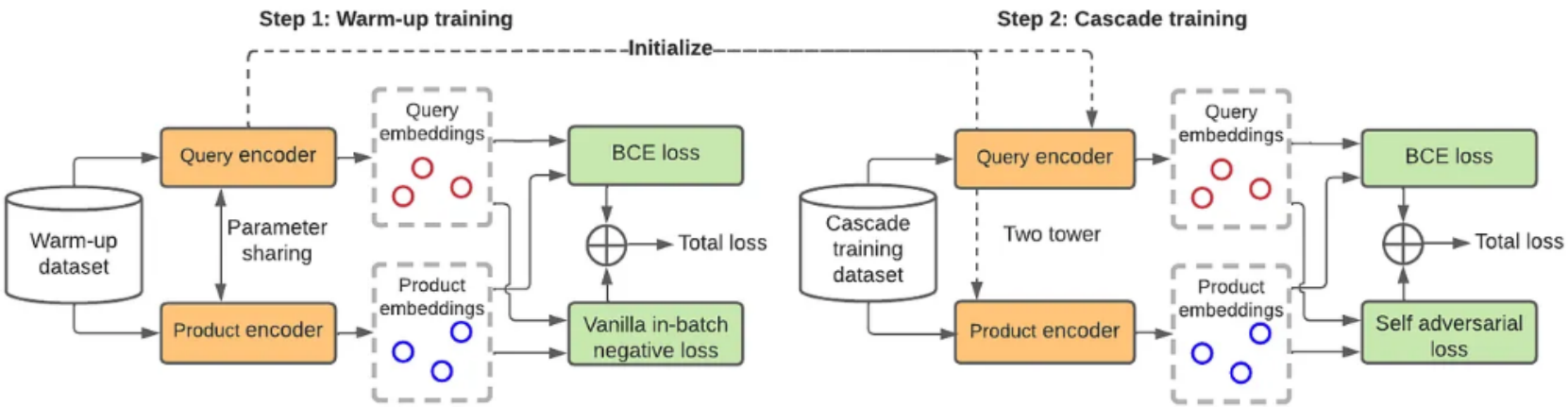


Figure 4. Two-step cascade training for ITEMS.

System Design

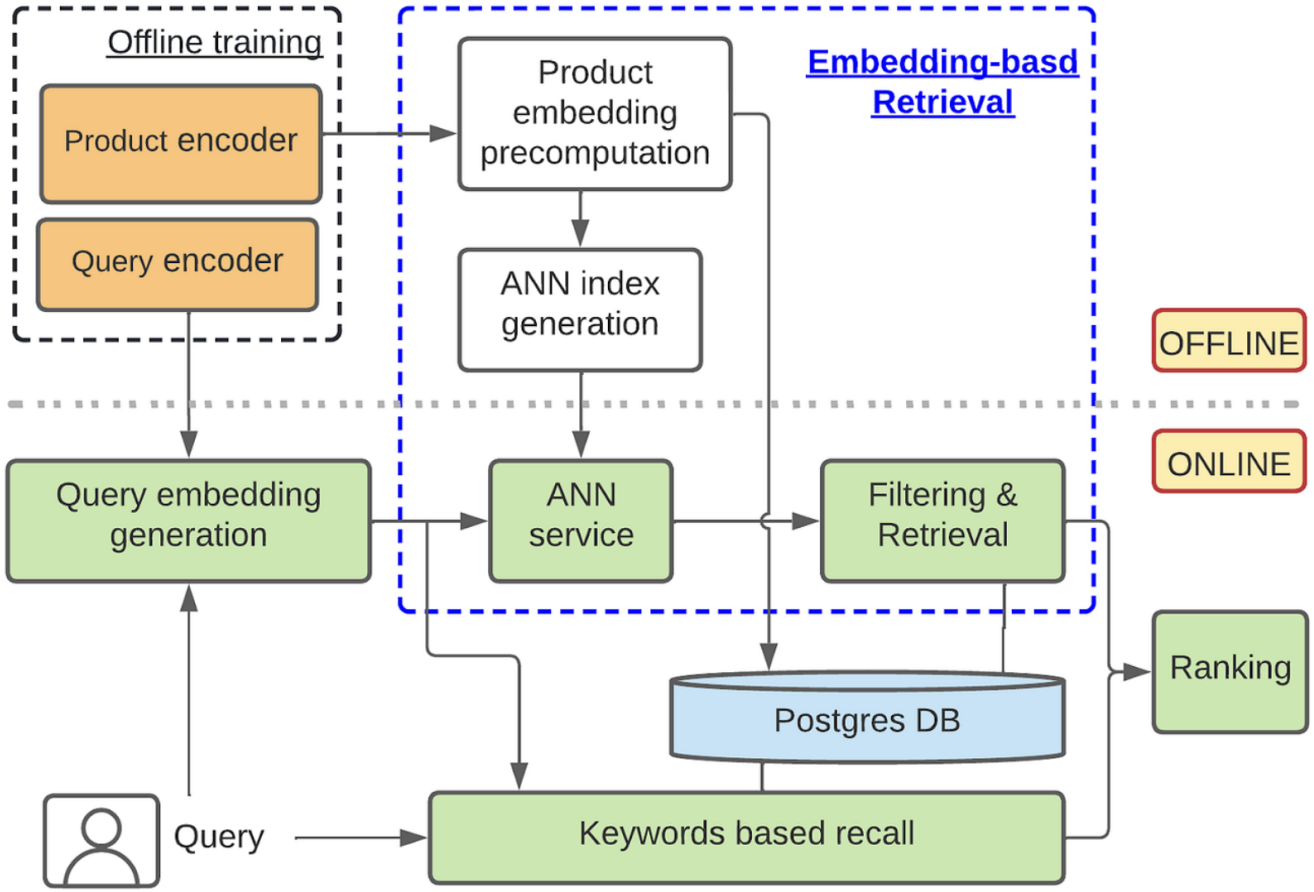


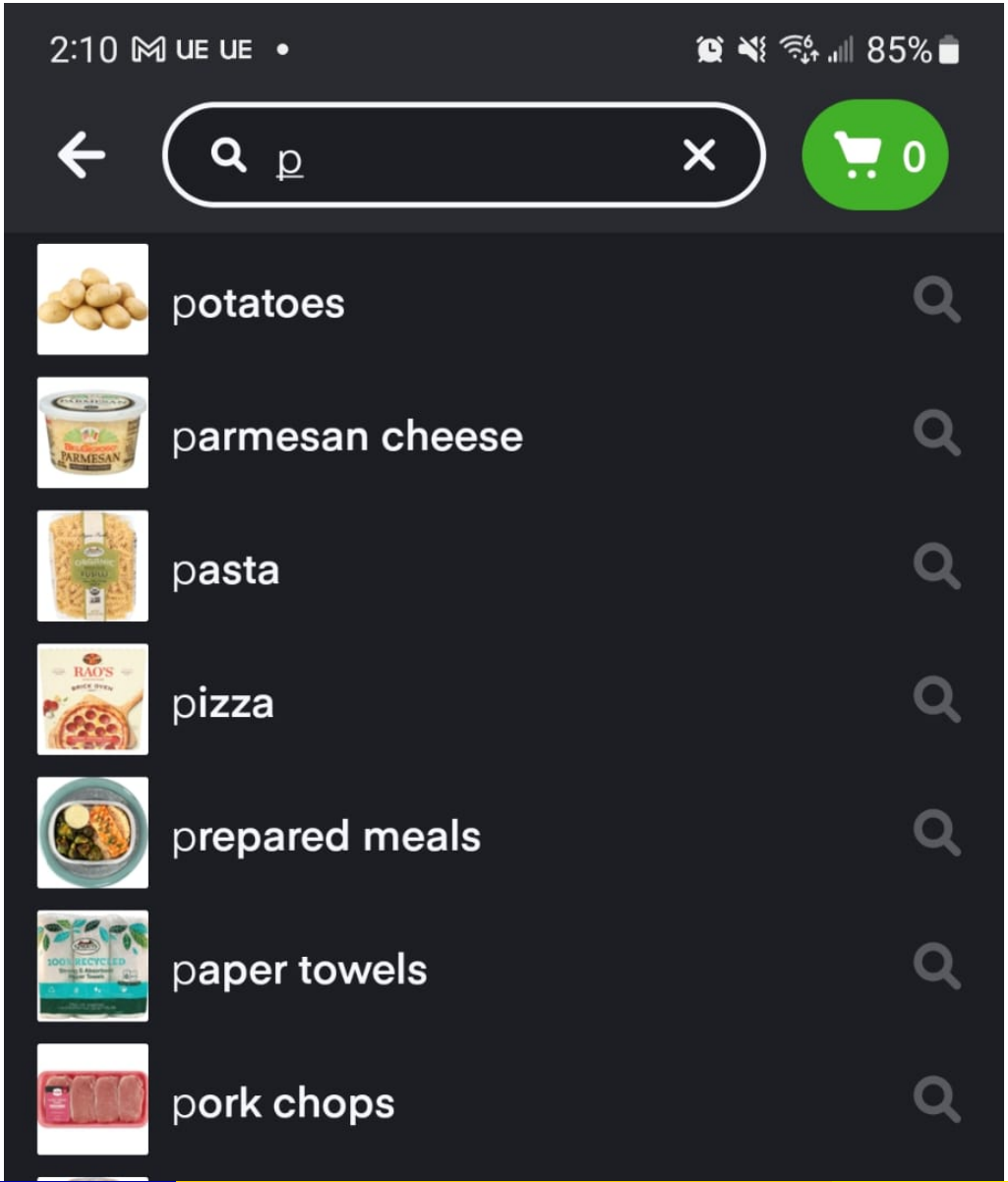
Figure 7. ITEMS system architecture.

Breakouts Time #1

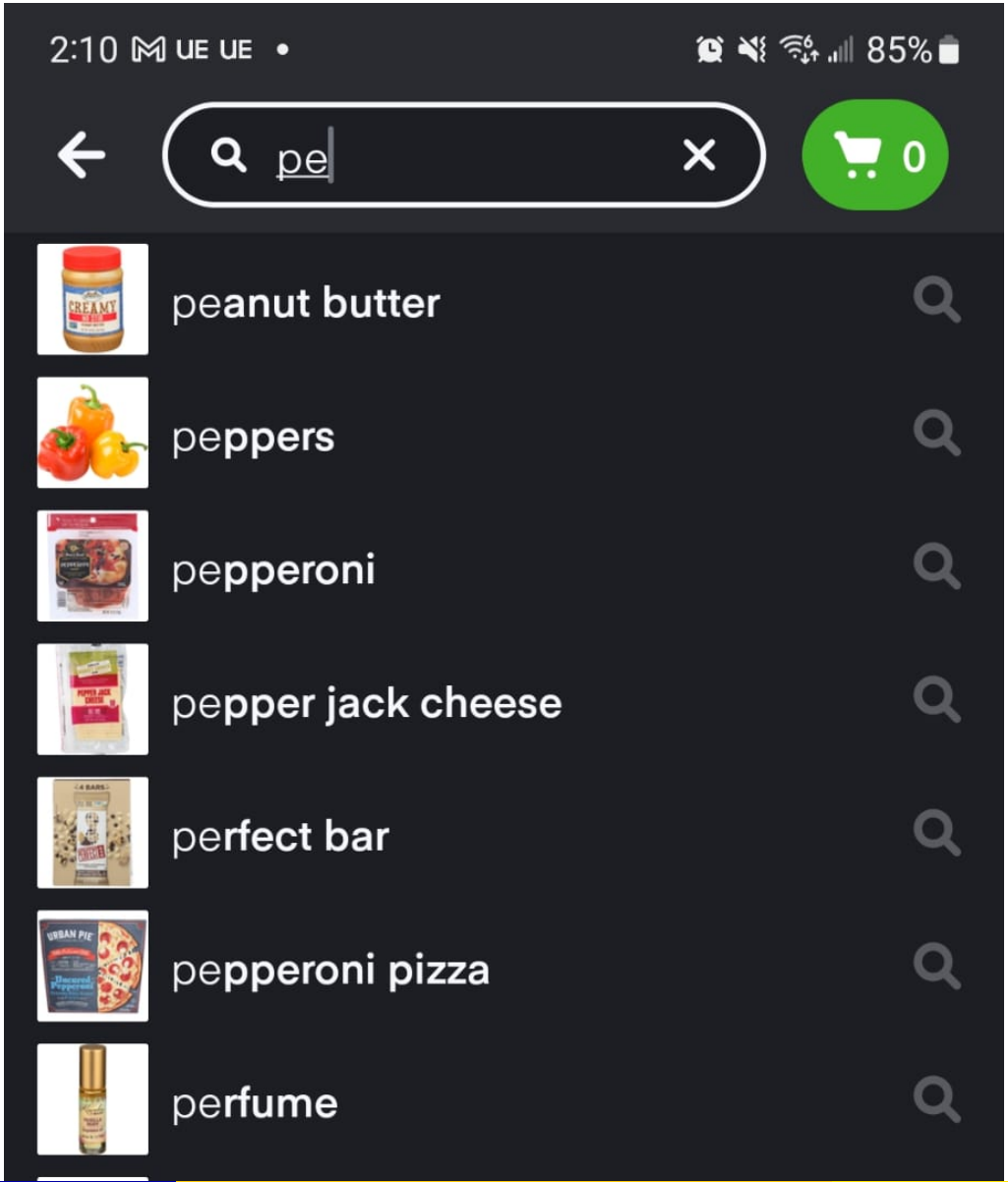
Auto-complete — 5 mins

Let's say you are tasked with building an in-email auto-completion application, which can help complete partial sentences into full sentences through suggestions (auto-complete). How would you use what we have learned so far to model this? What architecture would you use? What would be your data? And what are some pitfalls or painpoints your model should address?

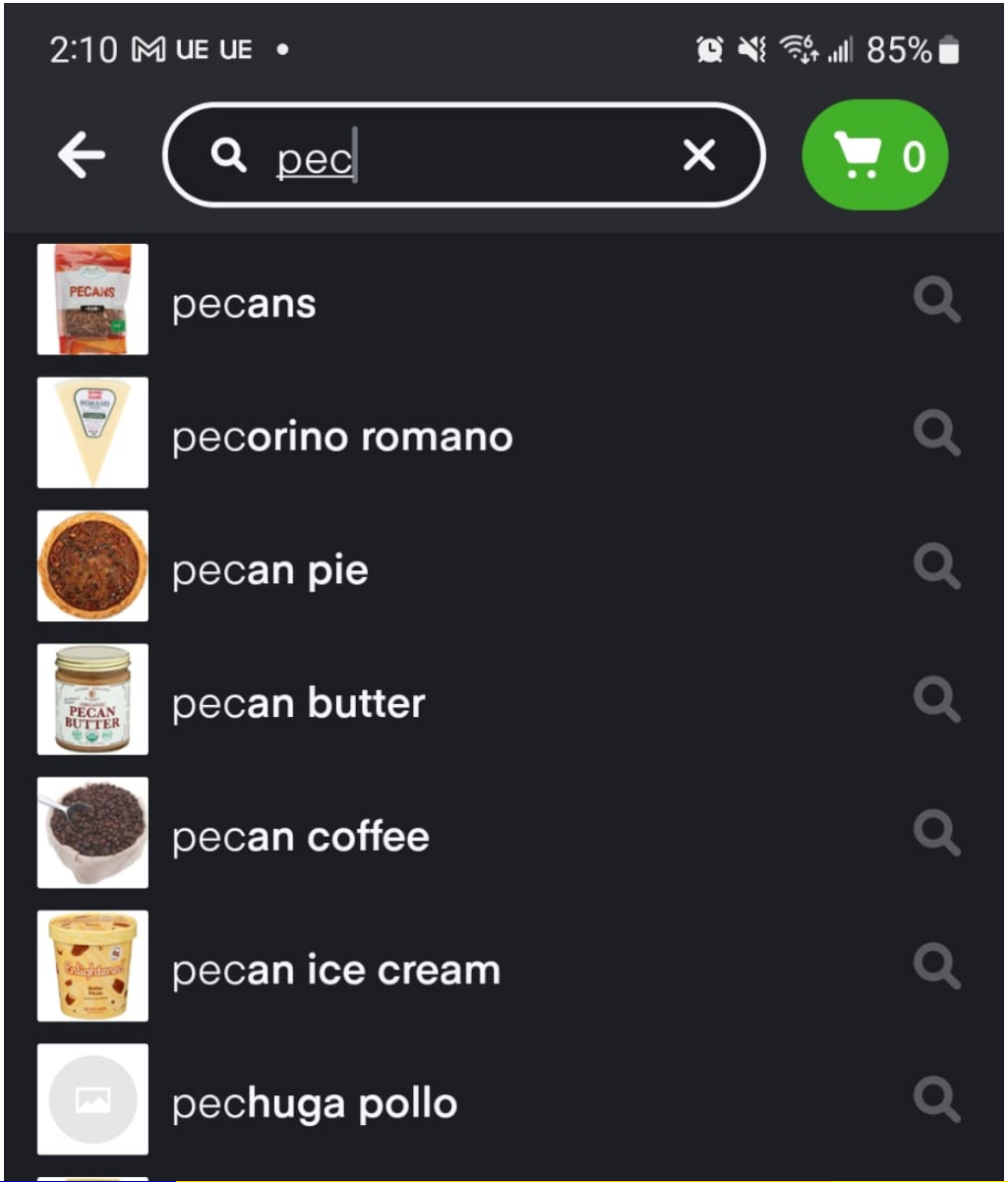
Instacart Auto-Complete and Search Relevance



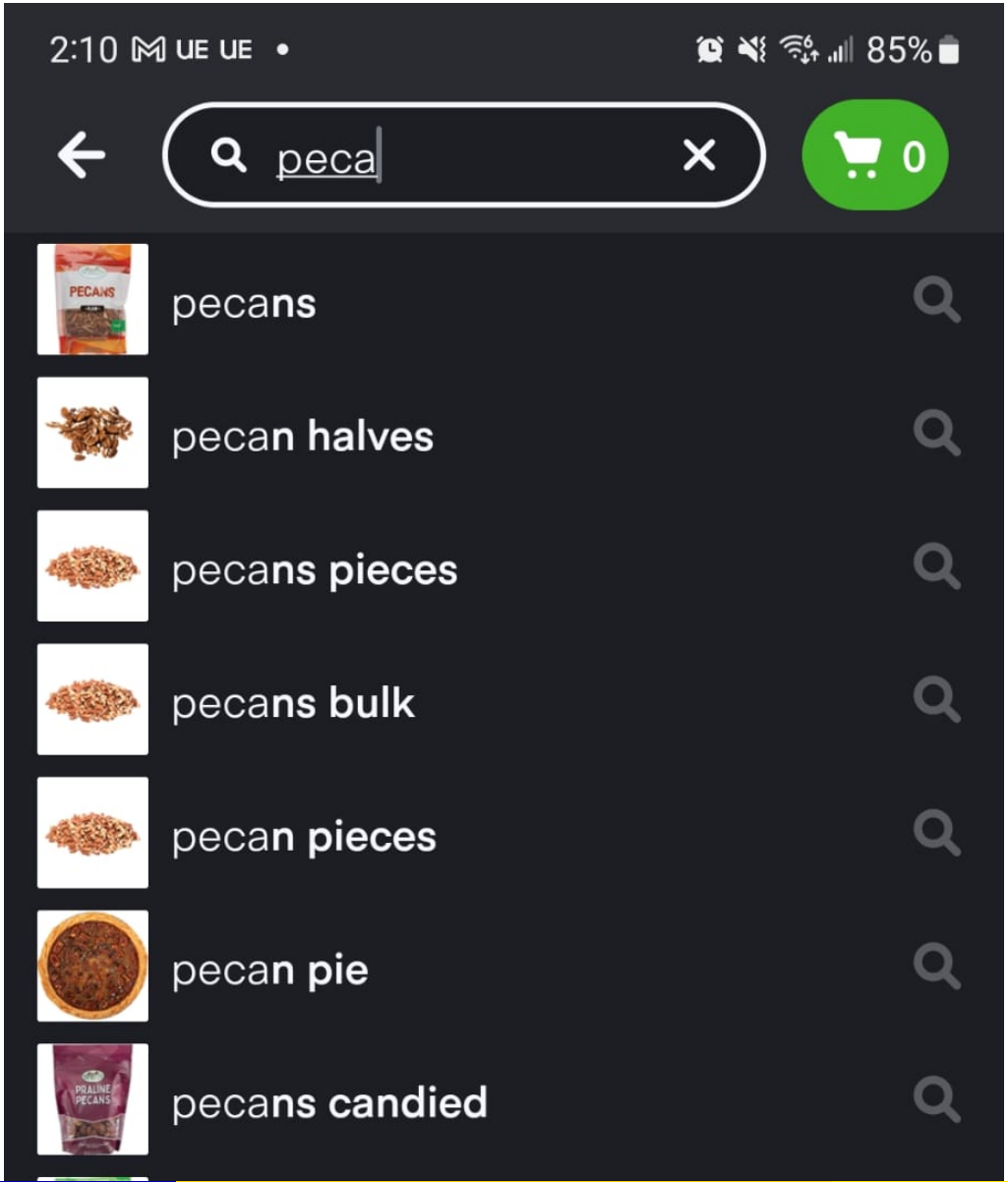
Instacart Auto-Complete



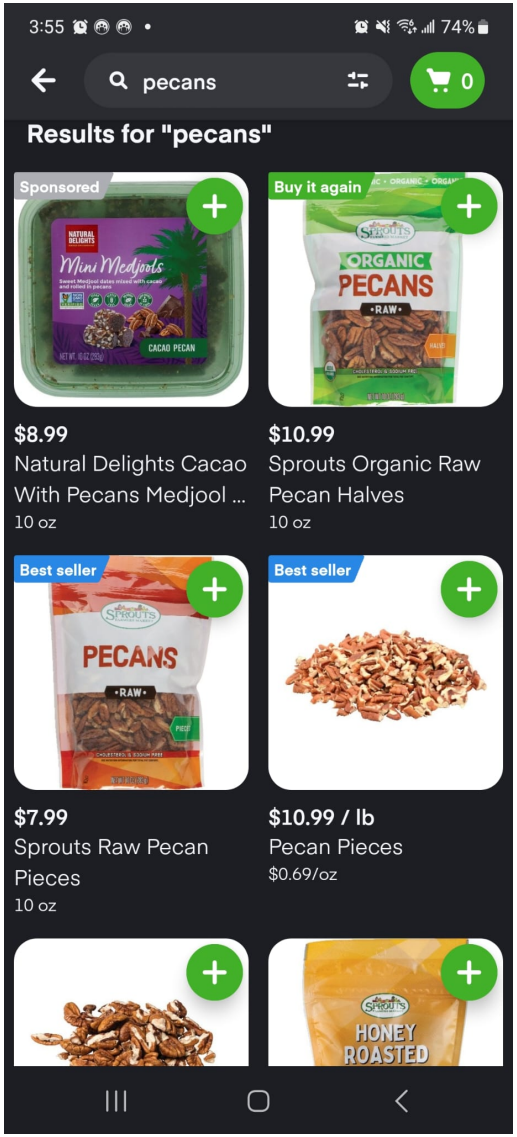
Instacart Auto-Complete



Instacart Auto-Complete



Instacart Auto-Complete and Search Results



Instacart Diversifying Auto-Complete

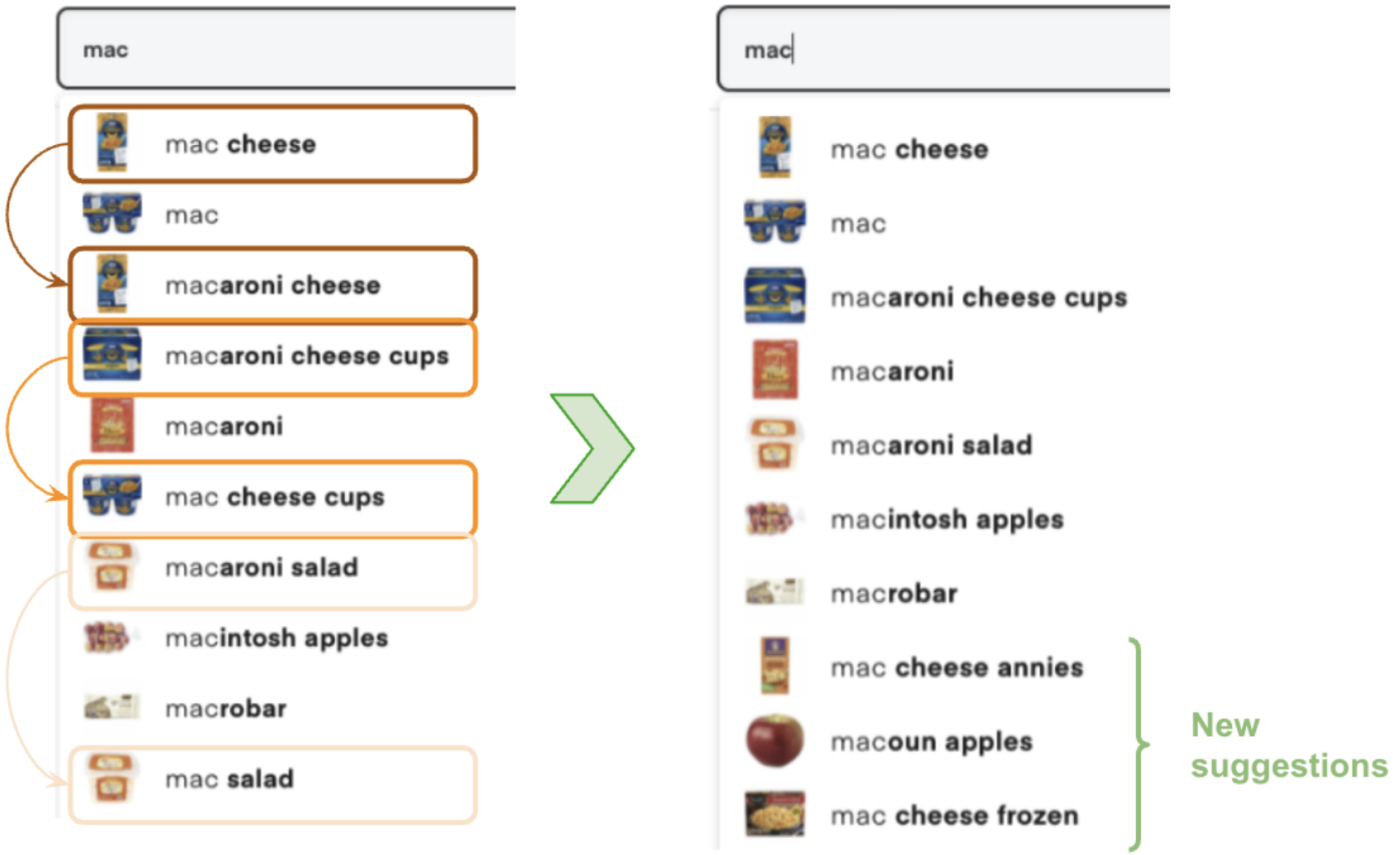


Figure 9. Autocomplete when a customer searches for “mac”, before (left) and after (right) semantic deduplication.