6.S079 LLMS IN A NUTSHELL

APRIL 2, 2024

MIKE CAFARELLA

Agenda

- Text Modeling
- Sequence Models
- Attention
- Transformers
- Fine-Tuning and RLHF

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The Core Thing

- We need a model that can compute P(someSentence)

- We can use it to build a sequence model
  - Input: a sequence of tokens
  - Output: a sequence of tokens

- Lots of applications can be built this way

Autoregressive Text Generation

- If you can compute P(nextWord | precedingWords)…
- P(nextWord | “My favorite food is”):
  - nextWord = “pizza”
  - nextWord = “love”
  - nextWord = “antagonist”
- Just try every possible word, pick the best

Autoregressive Text Generation

```
currentCtx = getUserInput()

while True:
    w = predictMostLikelyNextWord(currentCtx)
    emit(w)
    currentCtx += w

    if computeTerminationCriterion():
        break
```

Computing Sentence Probability

- For a sequence with n words
  $w^n_1 = w_1, w_2, \ldots, w_n$

- Every word w is drawn from a fixed vocabulary

- $P(w^n_1) = P(w_1)P(w_2|w_1)P(w_3|w^2_1)\ldots P(w_n|w^{n-1}_1)$
  $= \prod_{k=1}^{n} P(w_k|w_1^{k-1})$

Evaluation

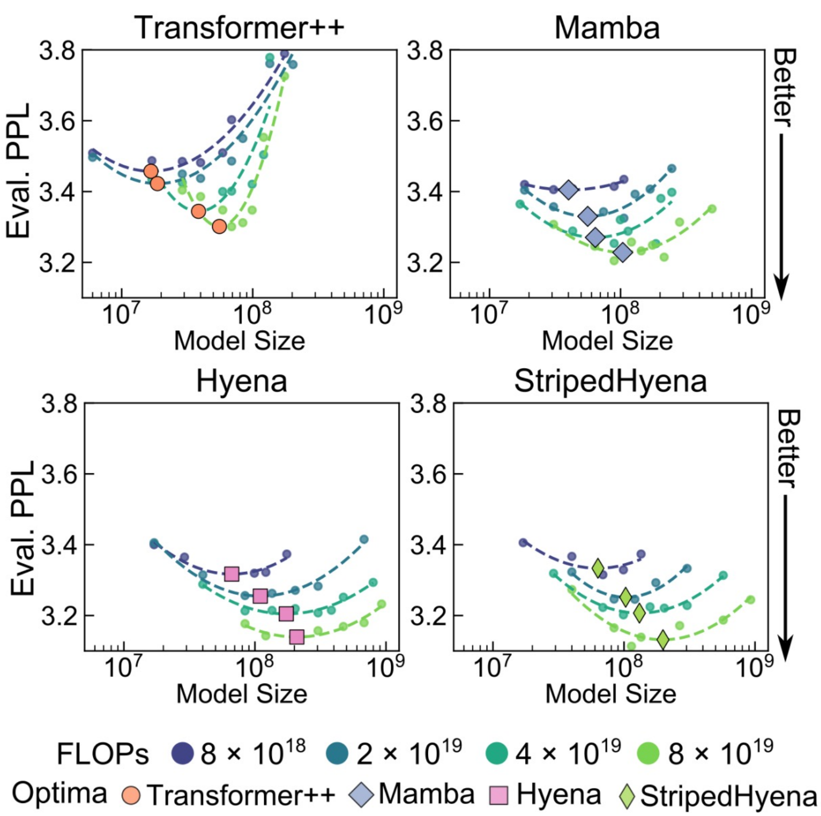
- How can we tell if the model is good?
  – Maybe it helps with a downstream task
  – A general-purpose metric would be nice

- "Perplexity" measures the inverse probability of an unseen test corpus with a particular language model
  – If text is real, then its probability should be high
  – Lower is better

$$PP(W) = P(w_1 \ldots w_N)^{-\frac{1}{N}}$$

Perplexity

- What's nice about Perplexity?
  - It's easy to compute
  - You don't need a concrete task
  - You don't need to understand the language!



Measures of Perplexity on different language models' predictions of single-nucleotide sequences from prokaryotic genomes

From Ngyuen et al, "Sequence modeling and design from molecular to genome scale with Evo", 2024

Perplexity

- What's bad about Perplexity?
  - It only works if your model gives a real probability (so: no rule-based methods)
  - Can't compare language models with different vocabularies
  - What is a "good" Perplexity number?

Data, Models, Features

- More context is better
- …but we will run out of data for statistics when k-grams get big enough

- We need some combination of:
  - More informative features
  - Constrained models to avoid overfitting
- …but feature engineering for language is extremely hard
- …and expressivity of the model is hard to engineer

Neural Methods

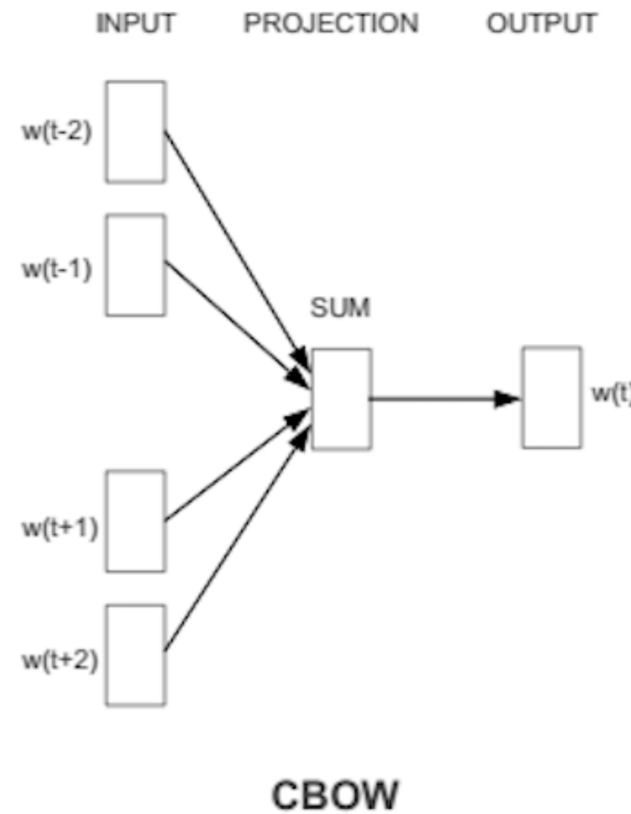
- Neural methods like CBOW let us avoid feature engineering
- Managing overfitting is poorly-understood but works in practice through model architecture, dropout, and other methods

Encoder-Decoders

- Most sequence models use Encoder-Decoder architecture
  - The encoder converts the input into a compressed embedding-style representation
  - The decoder converts an encoded representation back into the target language
- Nice qualities:
  - You can train them separately
  - You can mix/match them them for different input and output types
- word2vec has encoder/decoder architecture

Beyond w2v

- Remember CBOW? It aims to predict the output word given its context
- What's bad about this for chat?



Weaknesses of w2v for chat

- Input architecture "looks into the future" (this is easy to fix)
- Each word has a single embedding, regardless of usage
  - "I am going to **stick** to it"
  - "I am going to throw the **stick**"
  - The w2v embedding for stick will reflect both senses, even though in some contexts the correct sense is obvious to a human
- Can't handle truly huge vocabularies
- Sentence modeling is very primitive

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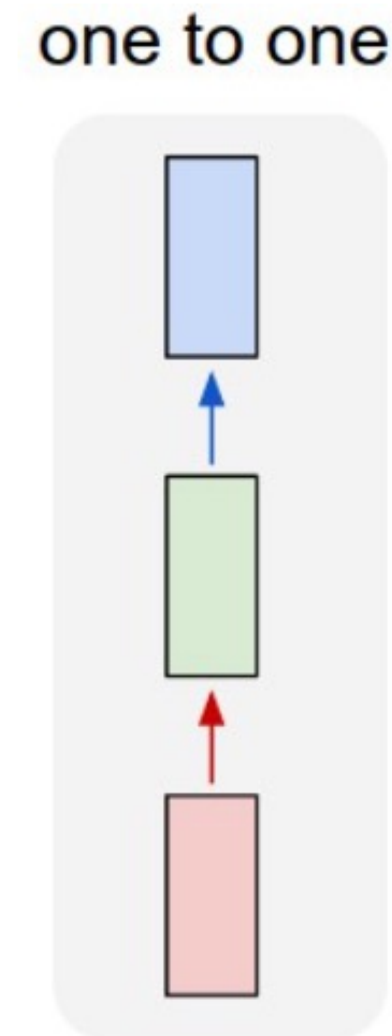
Sequence Modeling

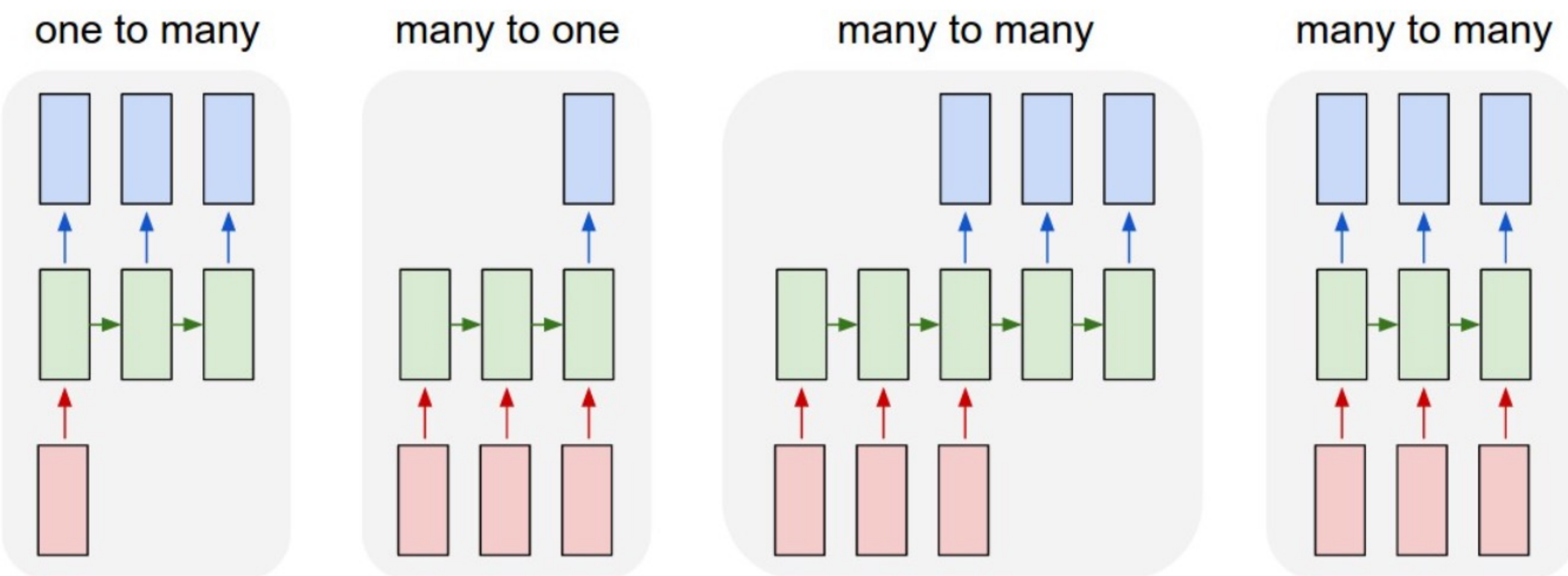
- The input/output model of w2v is really basic
  - You put in some fixed-size context
  - You get out a word
- What if input/outputs are variable length?
- What if they have complicated structure?



Images thanks to Karpathy, “Unreasonable Effectiveness of Recurrent Neural Networks”

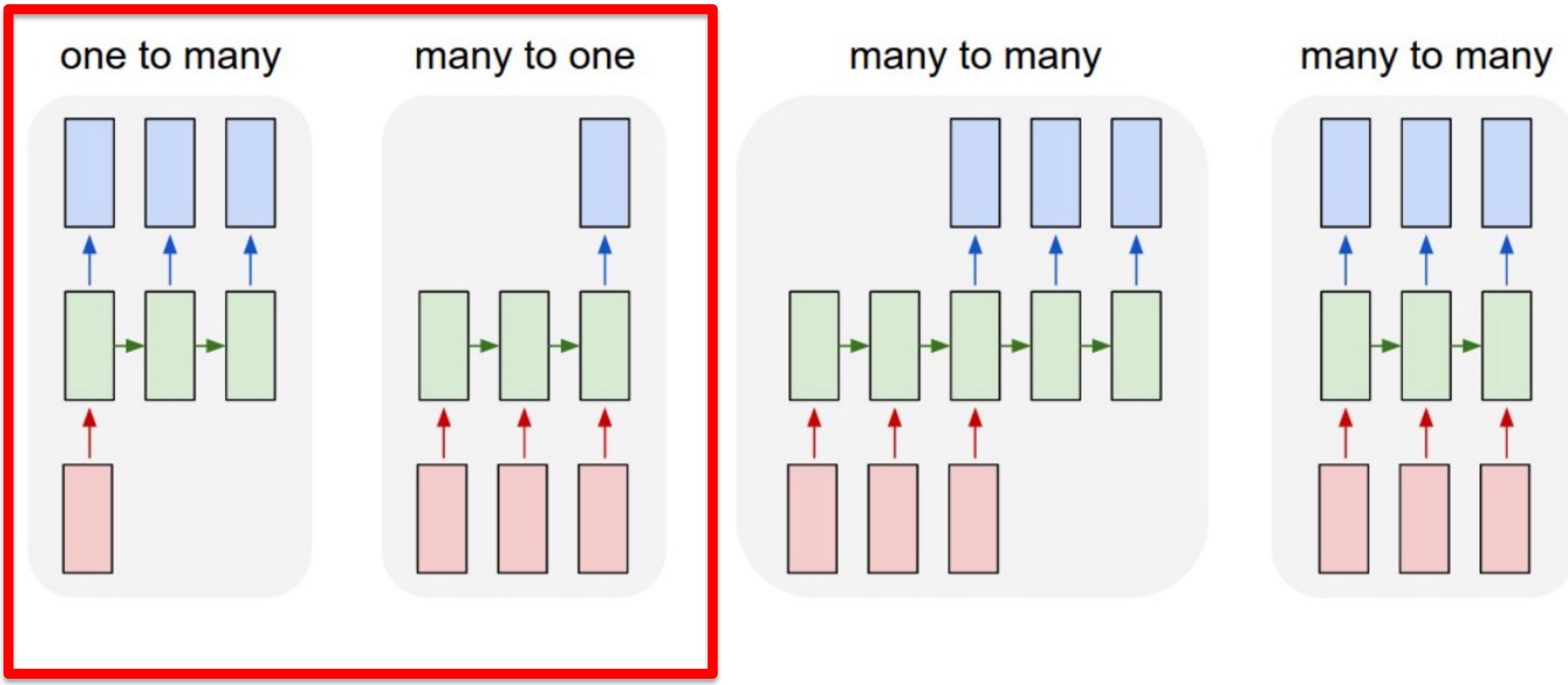
Sequence Modeling

- Sequence models offer more flexibility



- Red: input vectors, blue: output vectors
- **Green: internal state**

Sequence Modeling



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Sequence Modeling

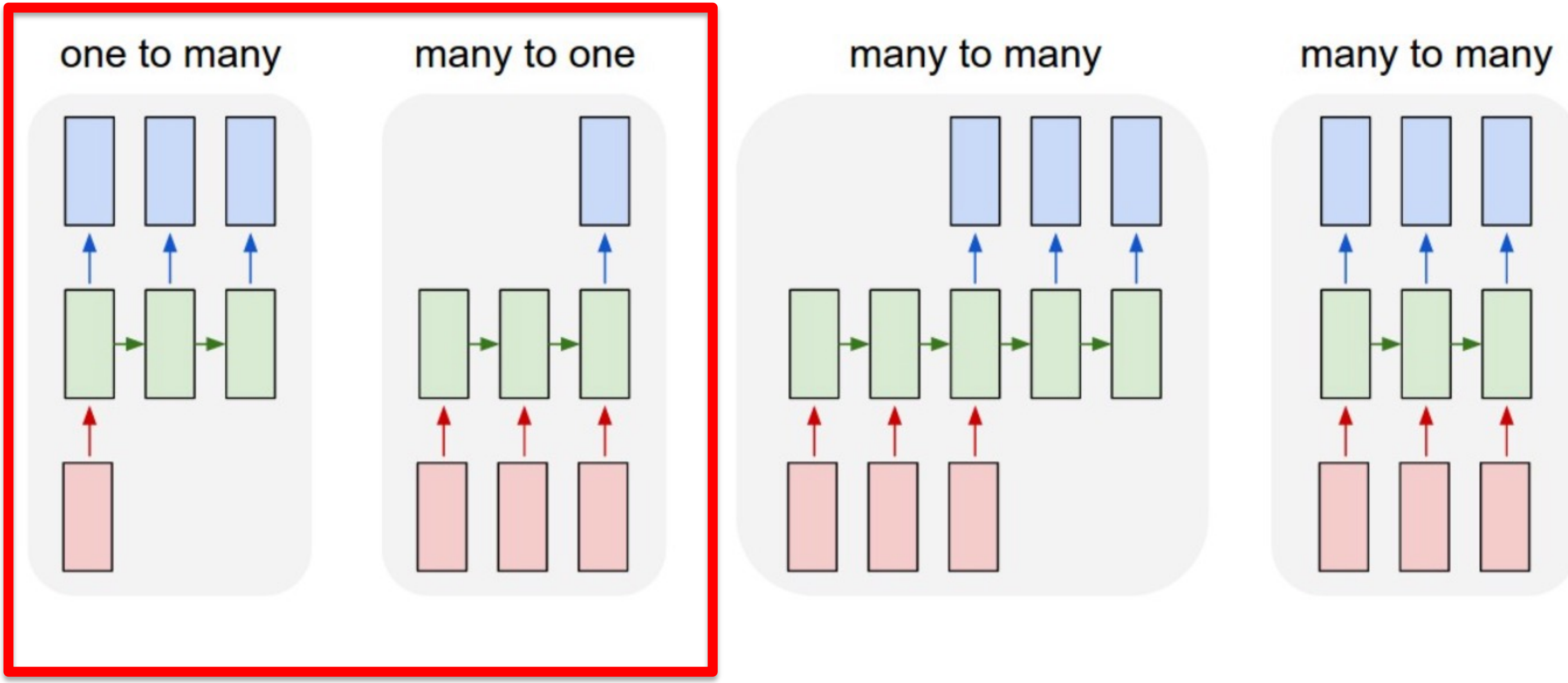
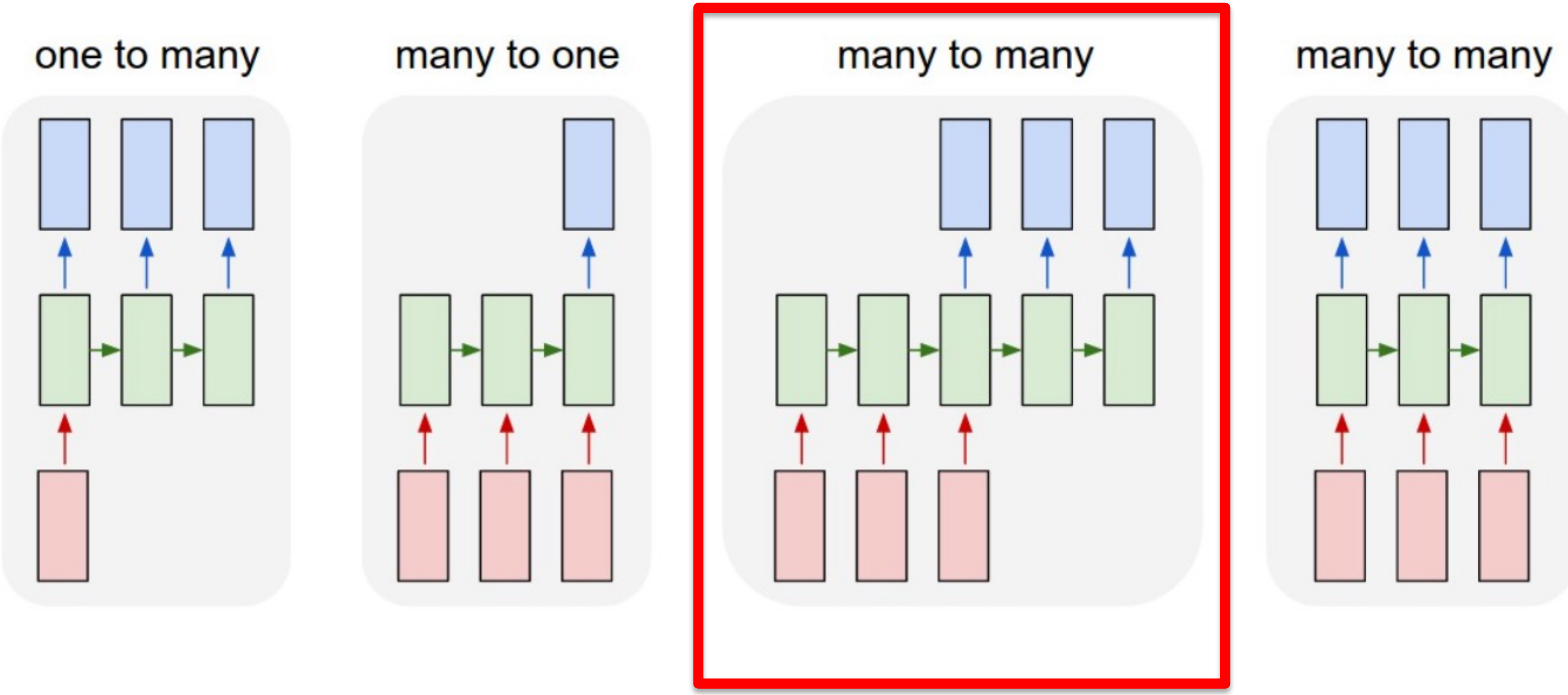


Image captioning

Text labelling

Sequence Modeling



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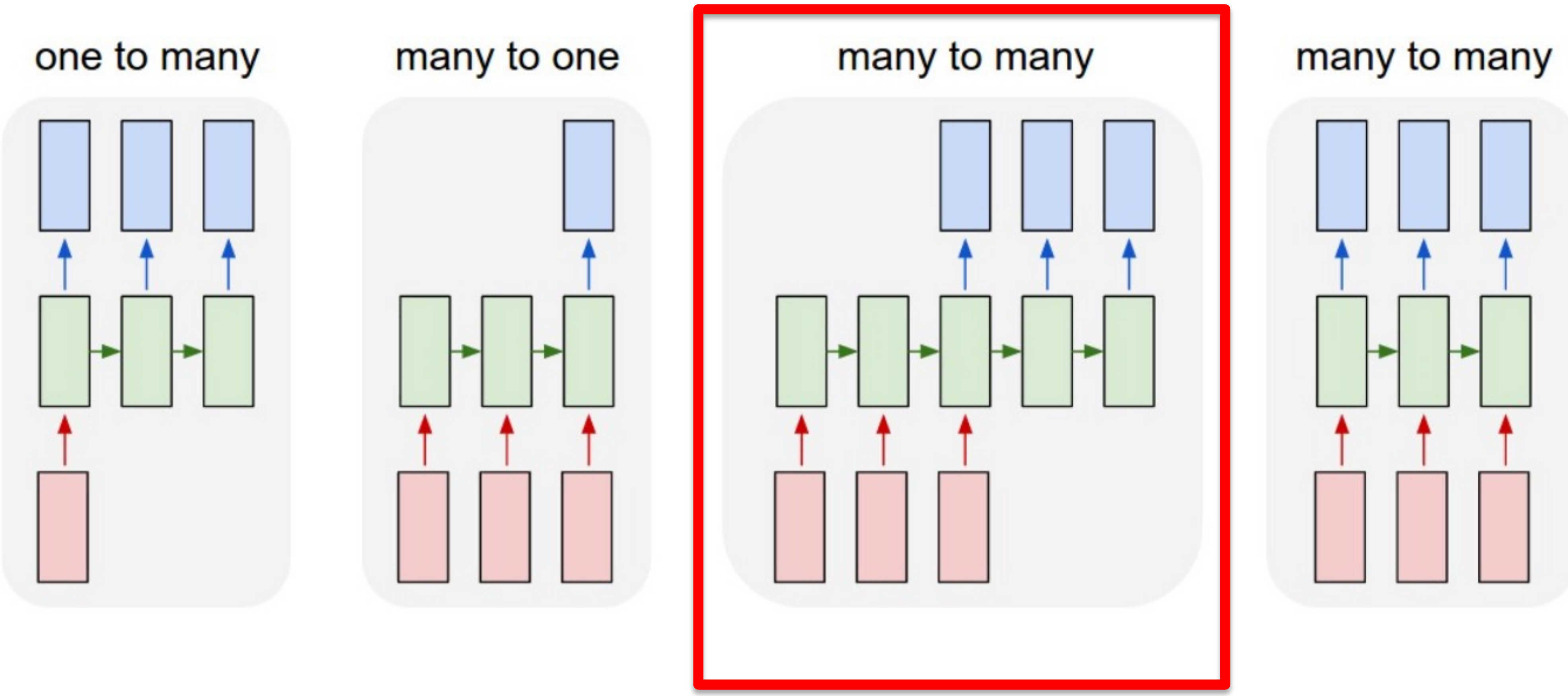
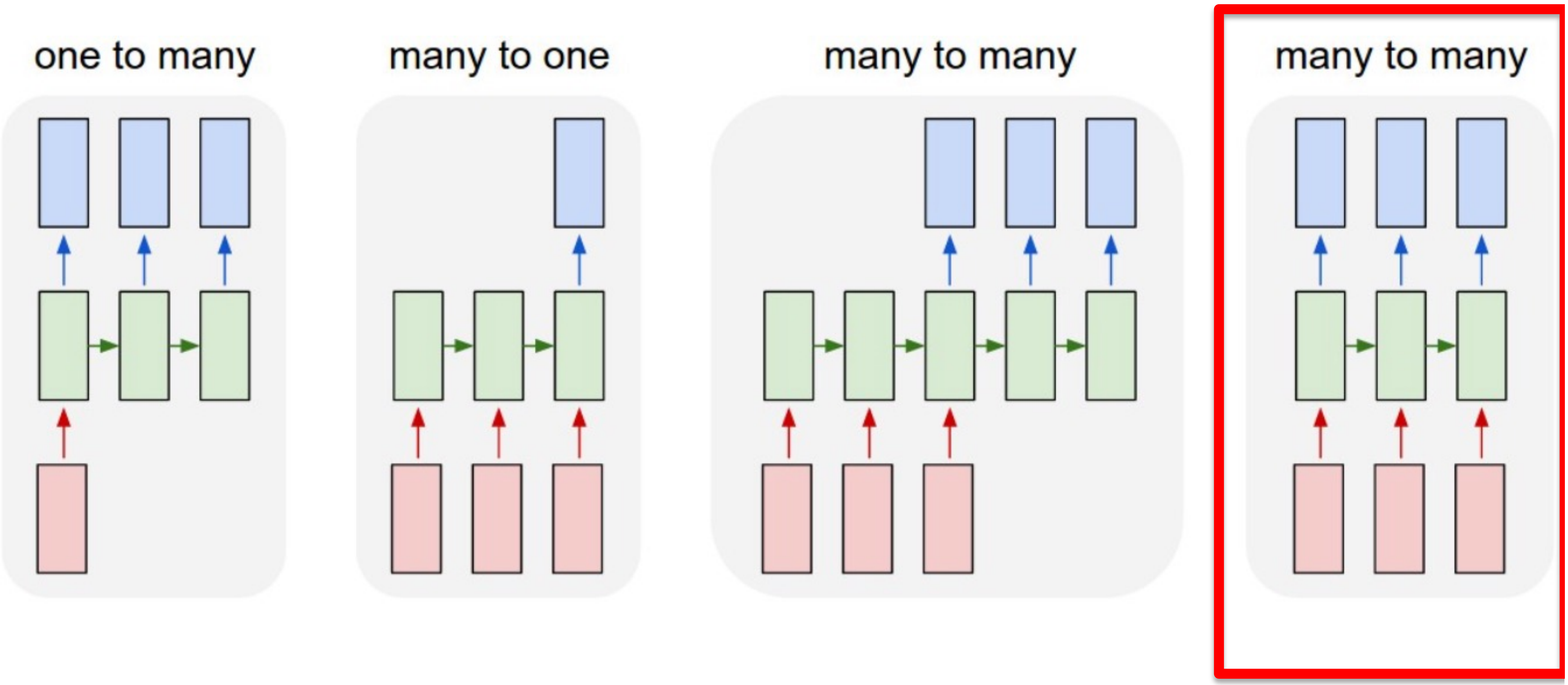
Sequence Modeling



Translation

Sequence Modeling



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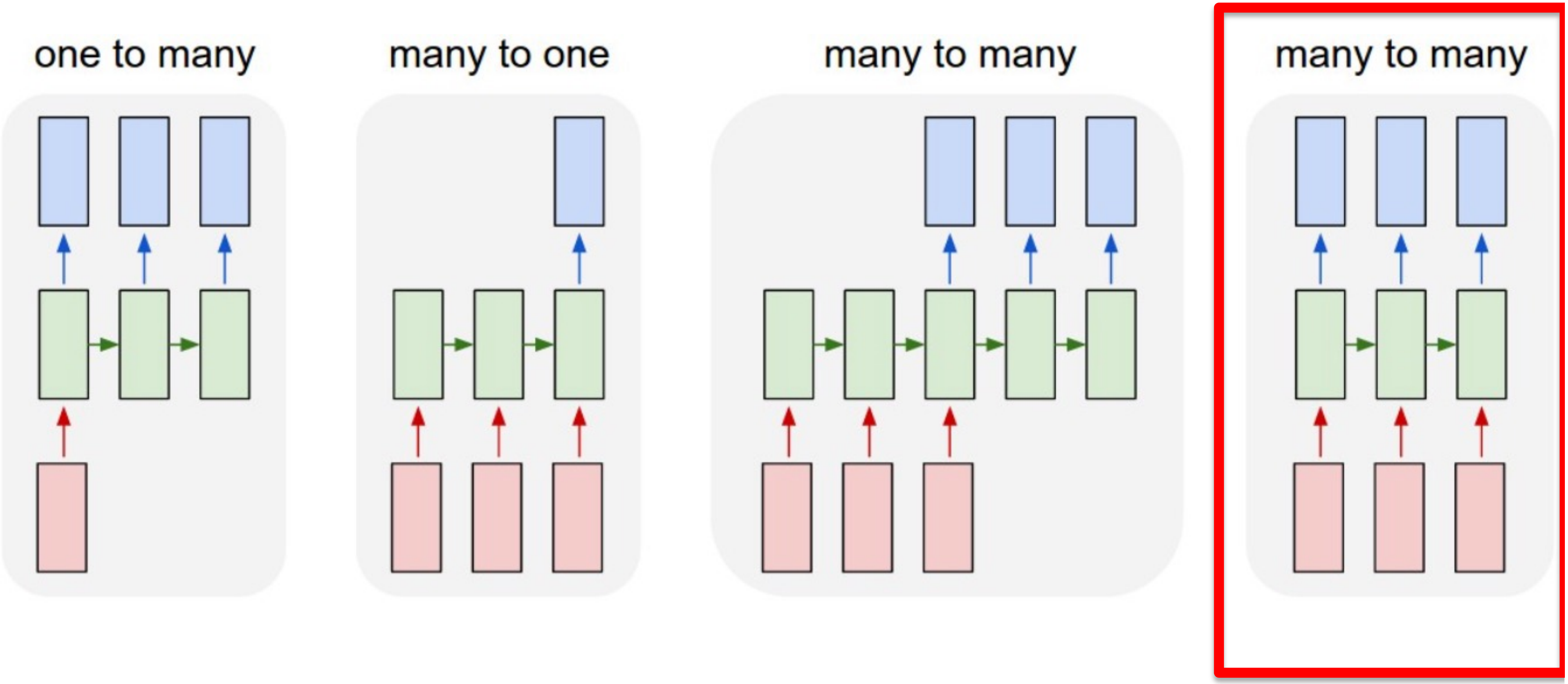
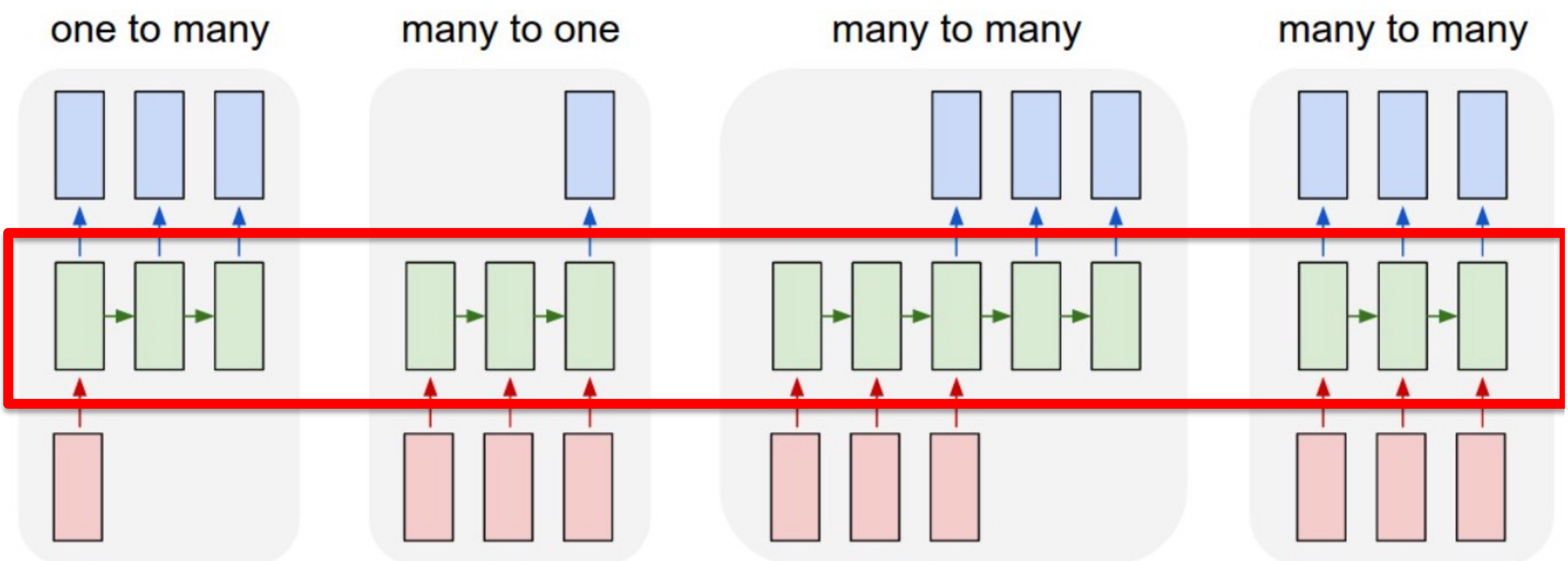
Sequence Modeling



Time-locked translation

(Hold off on chatbots for a bit...)

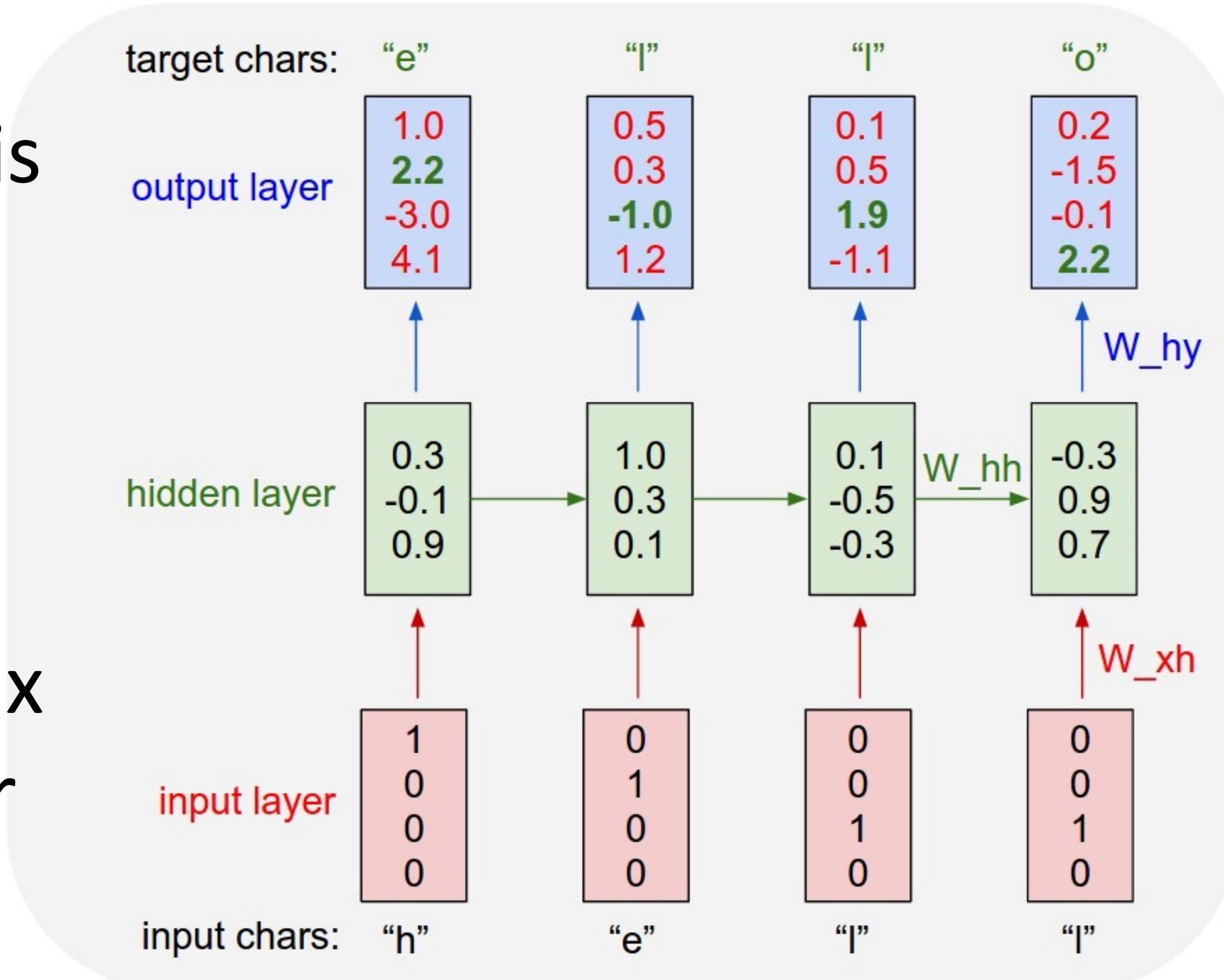
Sequence Modeling



- Internal state represents summary of inputs
- This breaks out of CBOB's fixed-size context
- Simplest version is a Recurrent Neural Network

Detailed View of Char Model

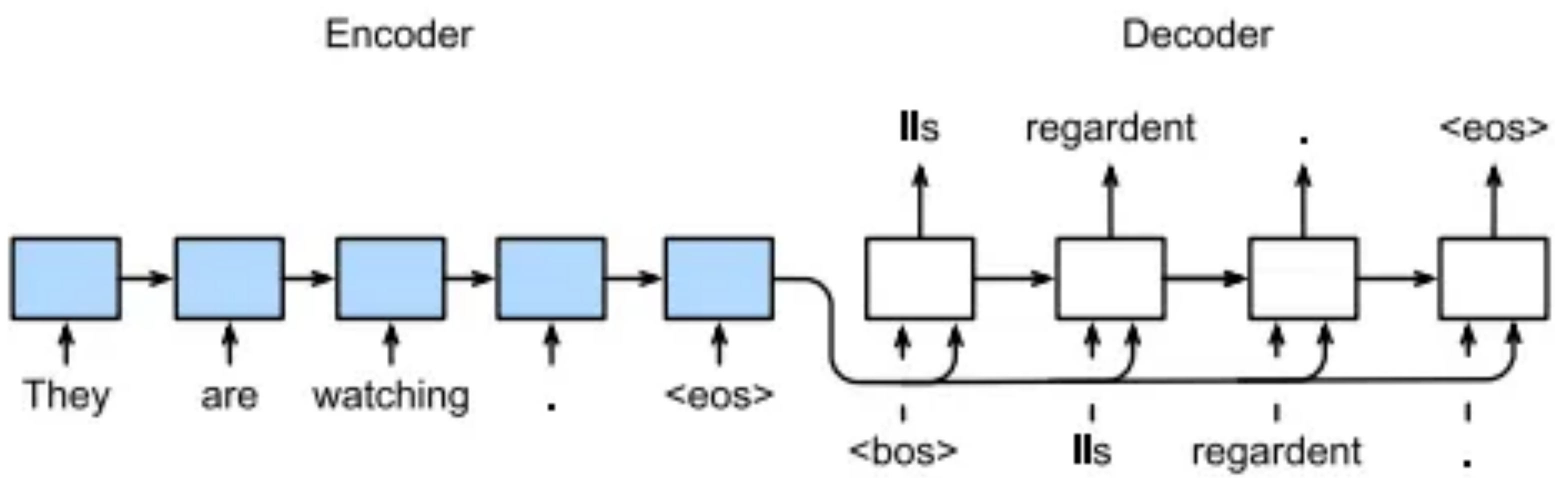
- Task: predict the next character
- One input word is broken into four "labeled" pairs
- Input is one-hot encoded
- Output is softmax prediction vector
- W_{xh} and W_{hy} are init'ed randomly, then learned via training



Karpathy, "Unreasonable …"

RNNs and seq2seq

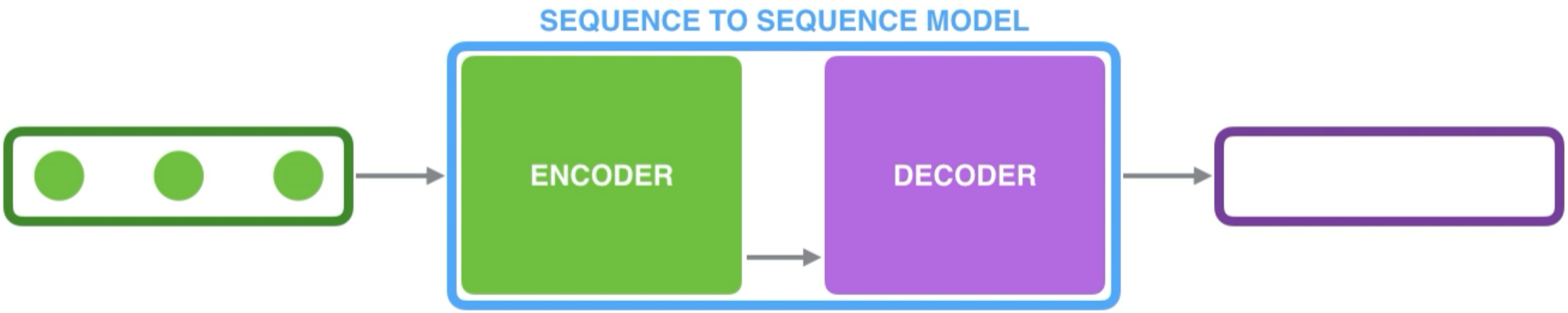
- Sometimes we have an entire sequence to translate, summarize, or answer
- We can train and combine two RNNs in an encoder/decoder “seq2seq” architecture



Sebastian Raschka, Vahid Mirjalili. Python Machine Learning

- Encoder RNN predicts next input. Decoder RNN takes encoder state and predicts next output

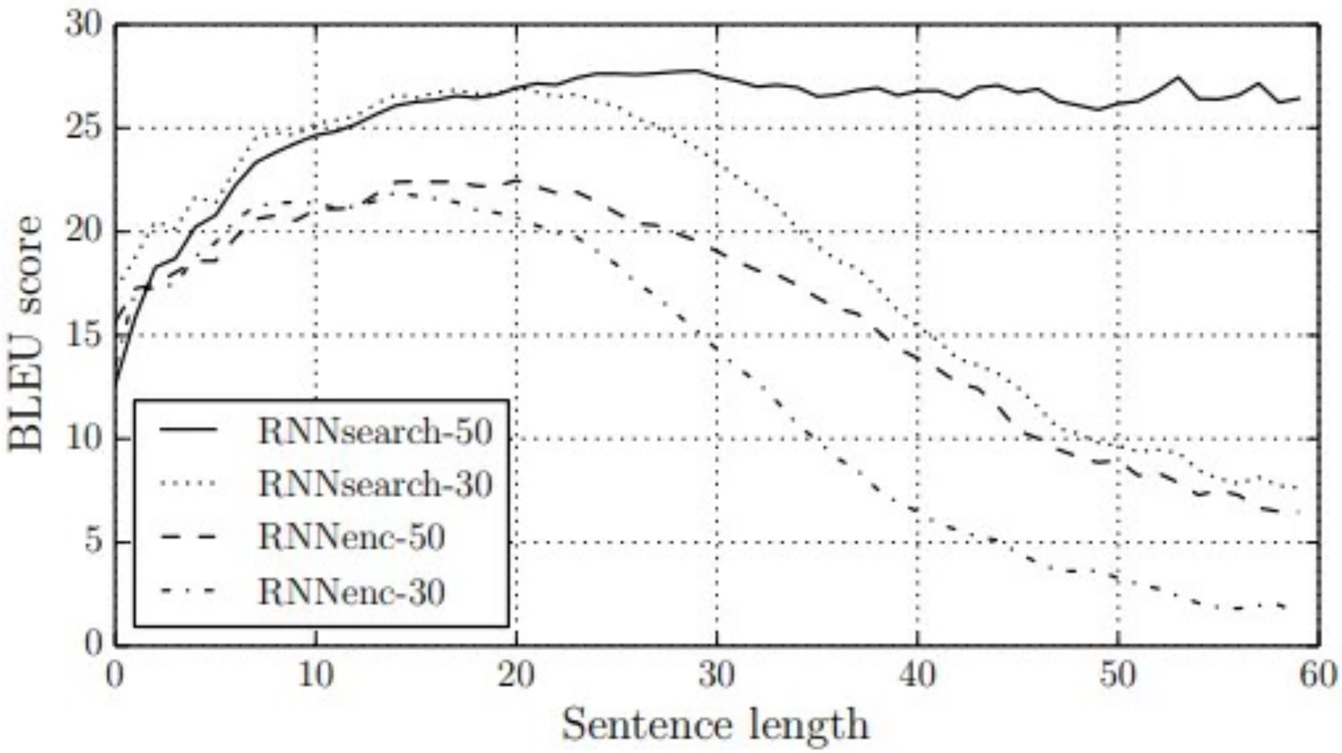
RNNs and seq2seq



Allamar, Visualizing A Neural Machine Translation Model

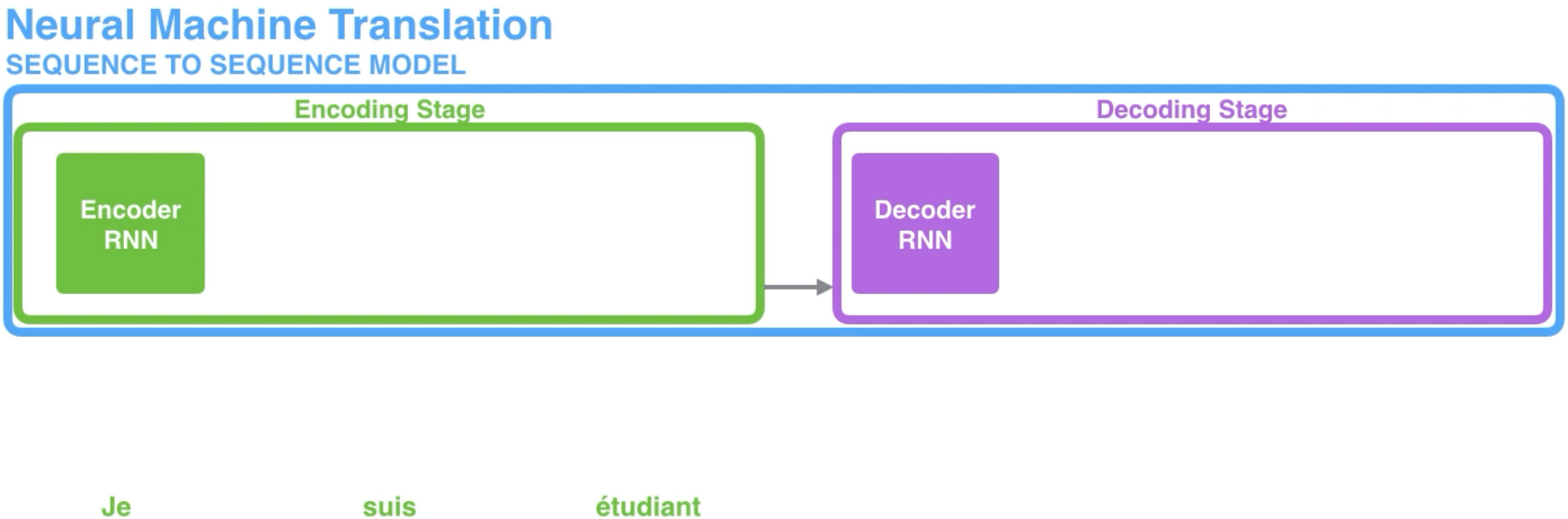
RNN Problems

- Long-distance information passing isn't great. First word of long seq may be "forgotten" by end
- In seq2seq architecture, the entire input sentence must be captured in one vector sent to decoder



Bahdanau, Cho, Bengio, "Neural Machine Translation By Jointly Learning to Align and Translate"

RNN Problems



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RNN Problems

- Long-distance information passing isn't great. First word of long seq may be "forgotten" by end
- In seq2seq architecture, the entire input sentence must be captured in one vector sent to decoder (the "encoder bottleneck")

- Various mechanisms invented to address this, such as Long Short-Term Memories
- LSTMs had trainable components to intentionally "forget" parts of input and alleviate bottleneck
- The "attention" mechanism was the most successful of these

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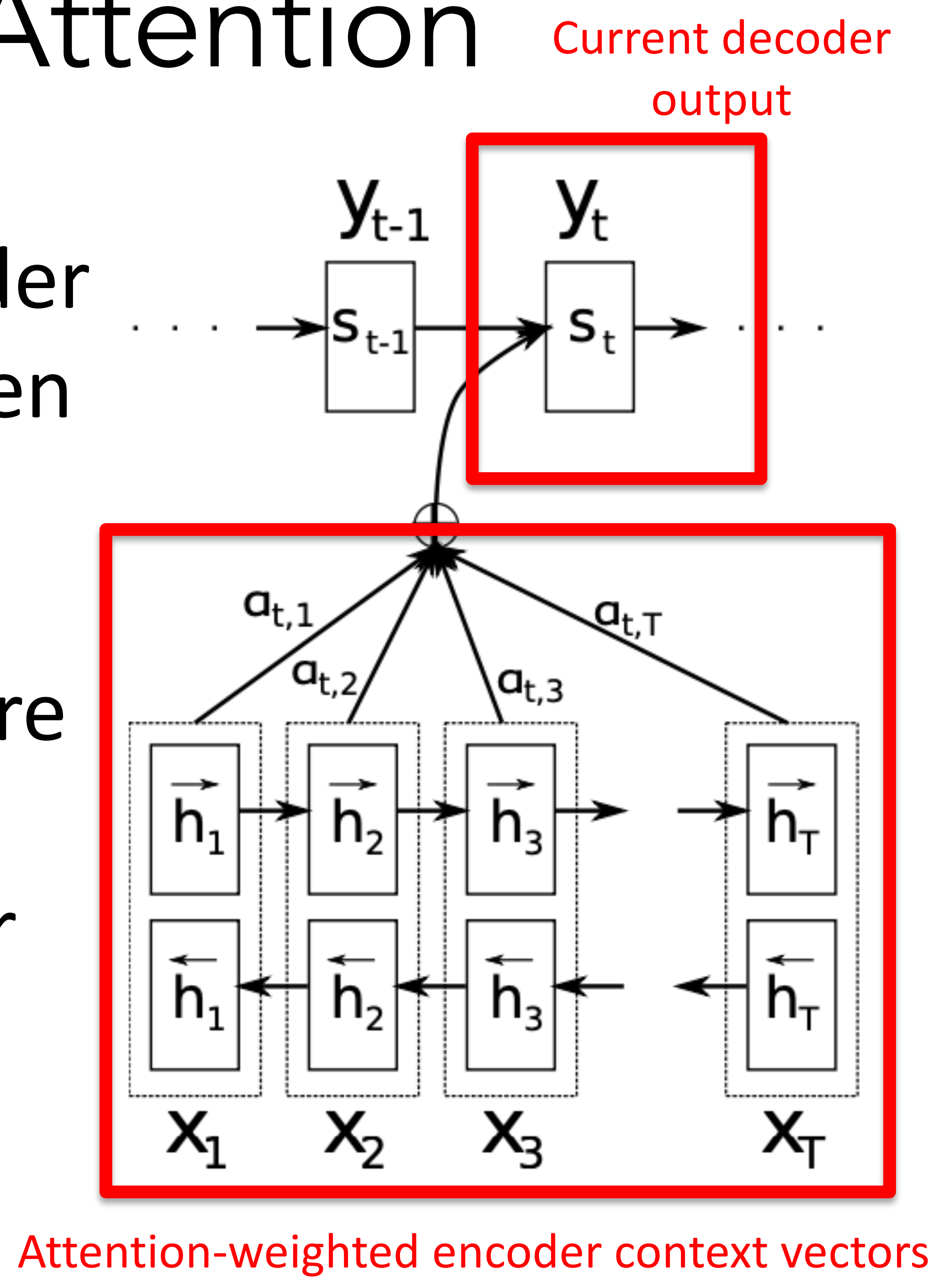
Paying Attention

- Core idea: given some input, figure out the important parts and (mainly) ignore the rest
- How does your attention work when reading?

- **The attention mechanism itself should be learned**
- First introduced in "Neural Machine Translation By Jointly Learning to Align and Translate", by Bahdanau, Cho, Bengio
- The decoder "chooses a subset of [encoder input] vectors adaptively while decoding the translation"

Bahdanau Attention

- Karpathy, AI's bard: "The context vector from encoder is a weighted sum of hidden states of words of the encoding"
- Those attention weights are themselves computed by looking at current decoder state and encoder values



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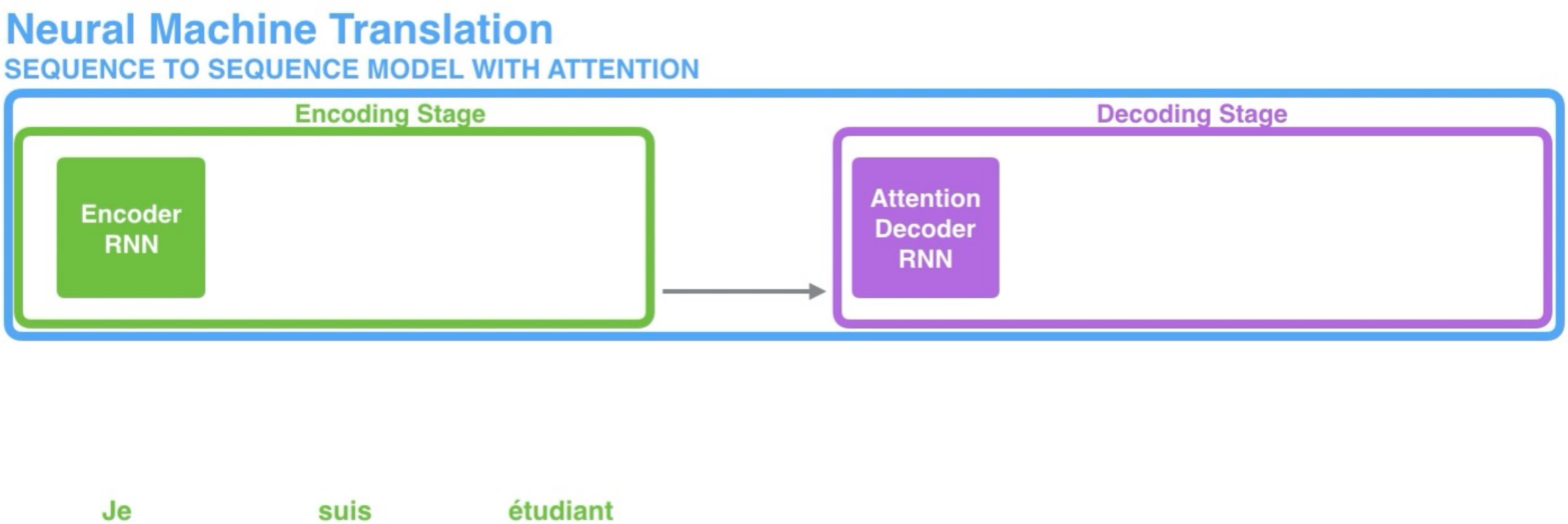
Bahdanau Attention

Allamar, Visualizing A Neural Machine Translation Model

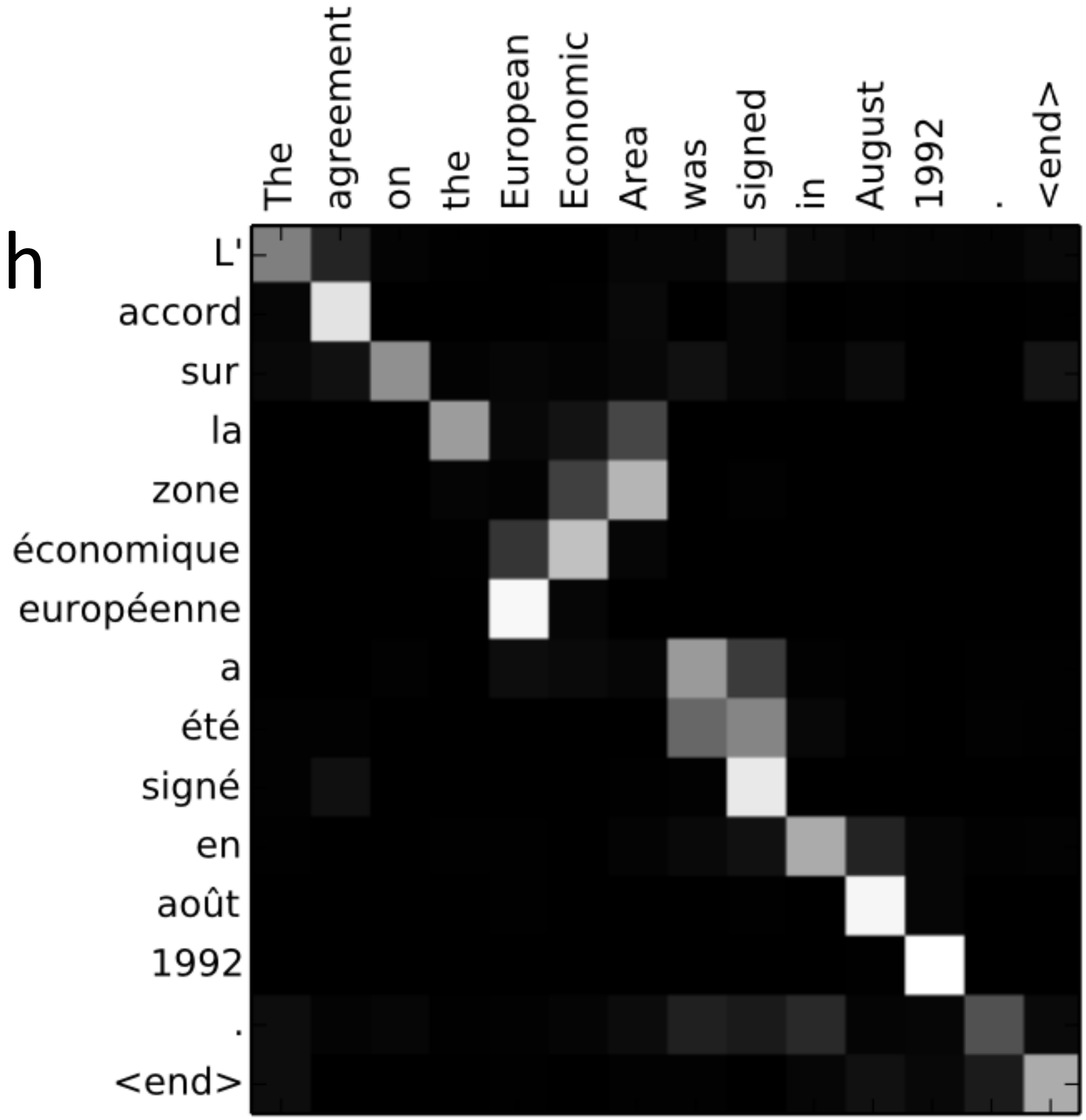
Bahdanau Attention



Allamar, Visualizing A Neural Machine Translation Model

Attention Visualization

- Consider translating English to French
- Pixel values indicate relevance of input word to output word



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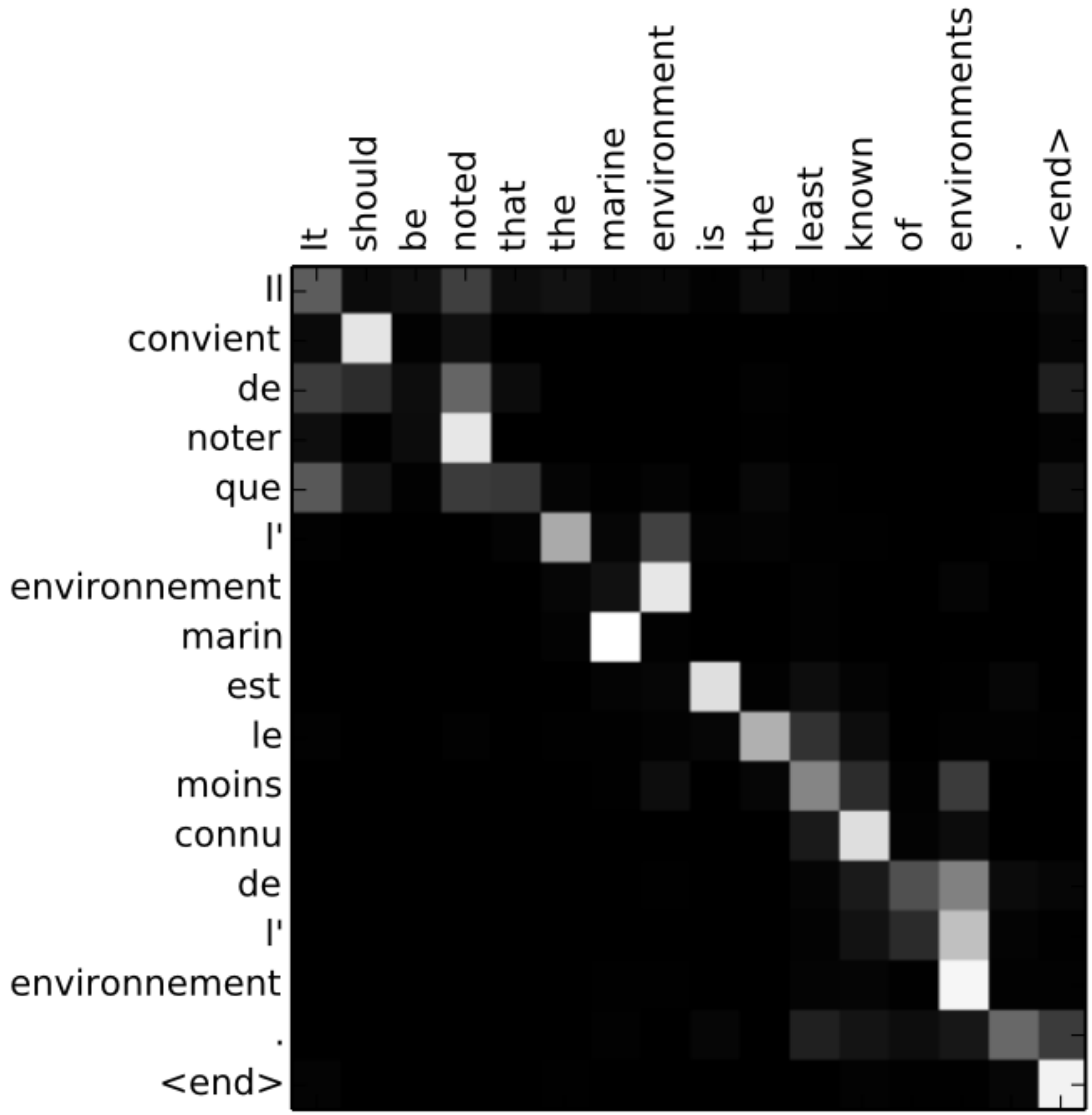

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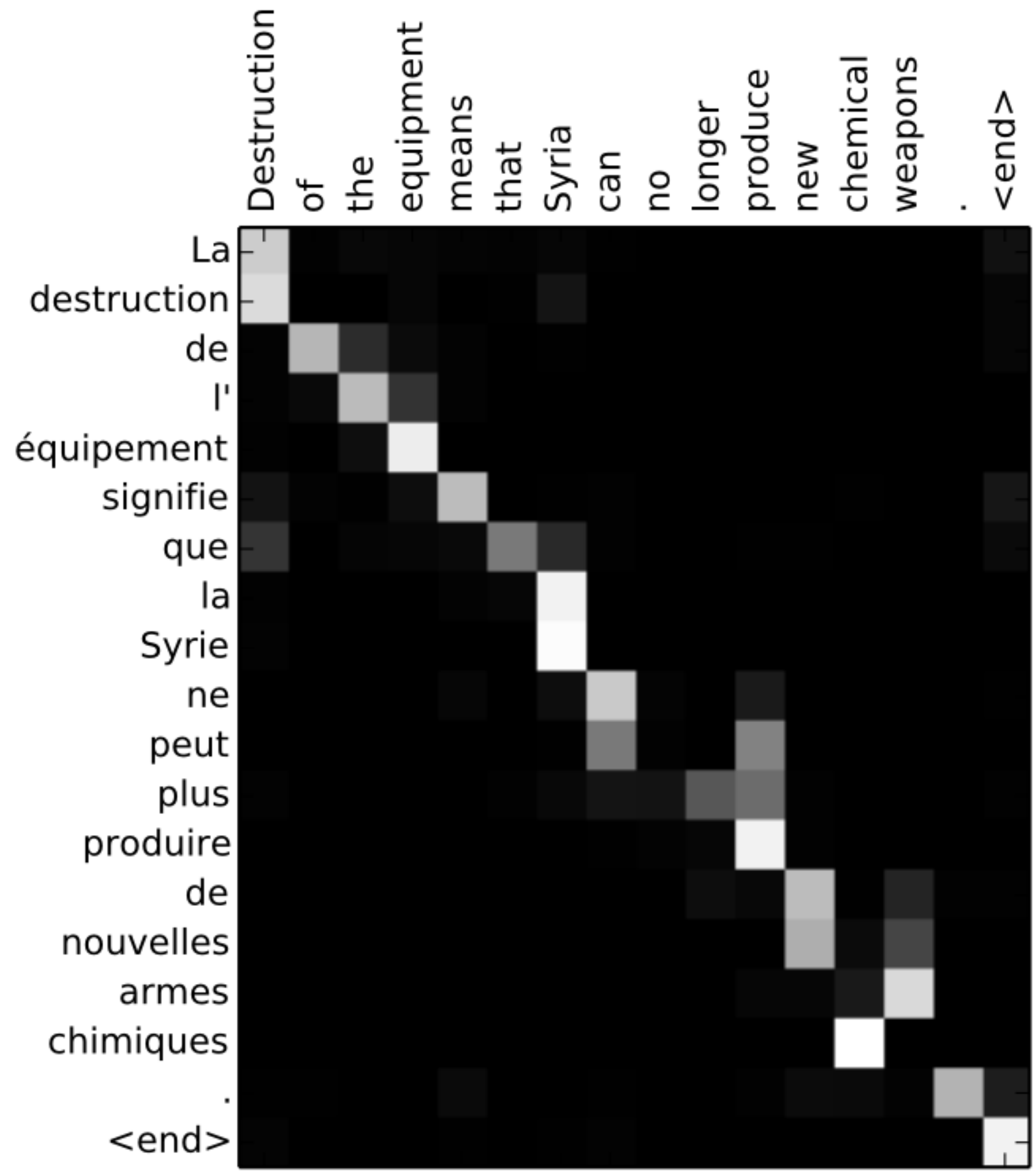

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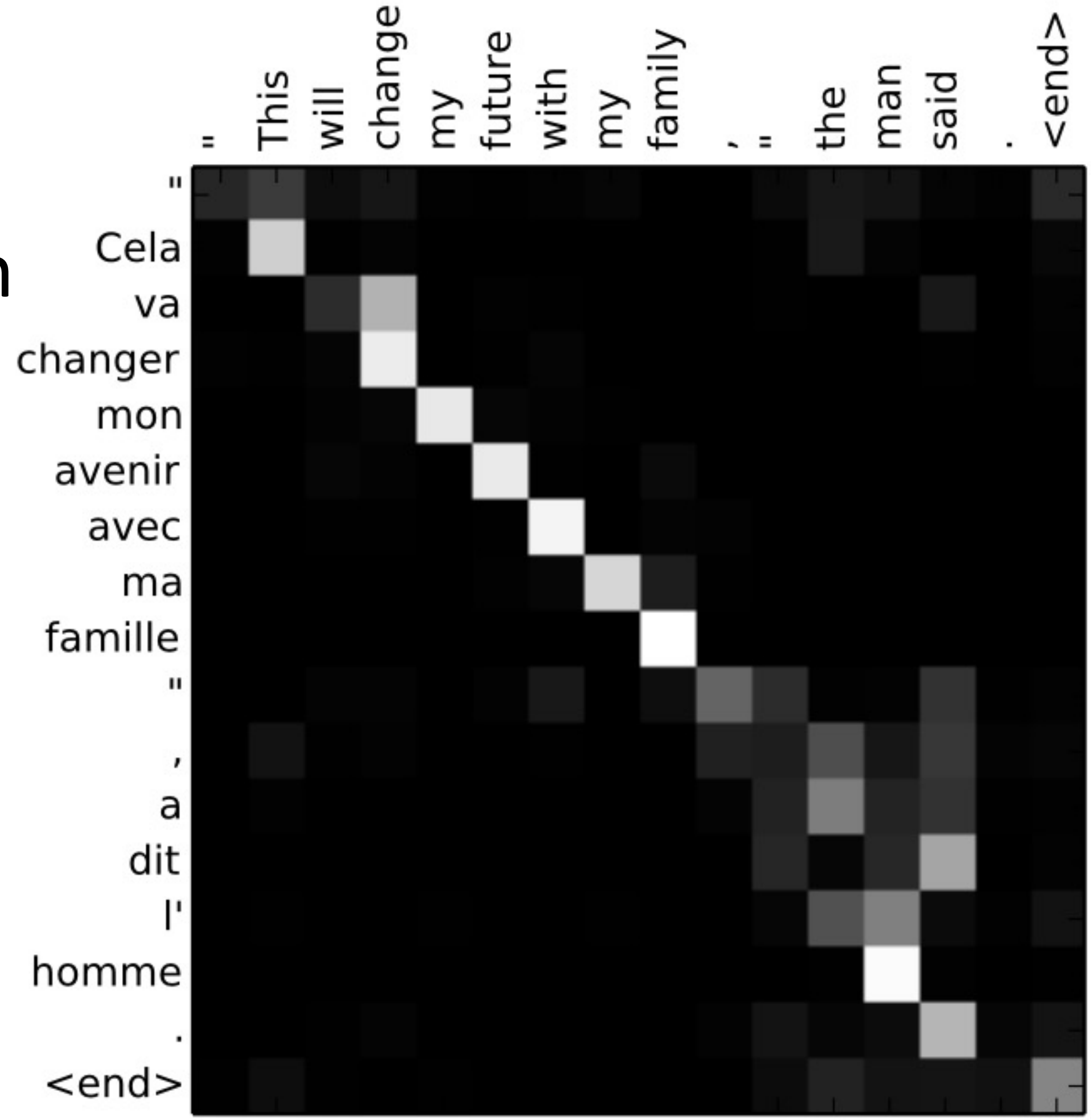
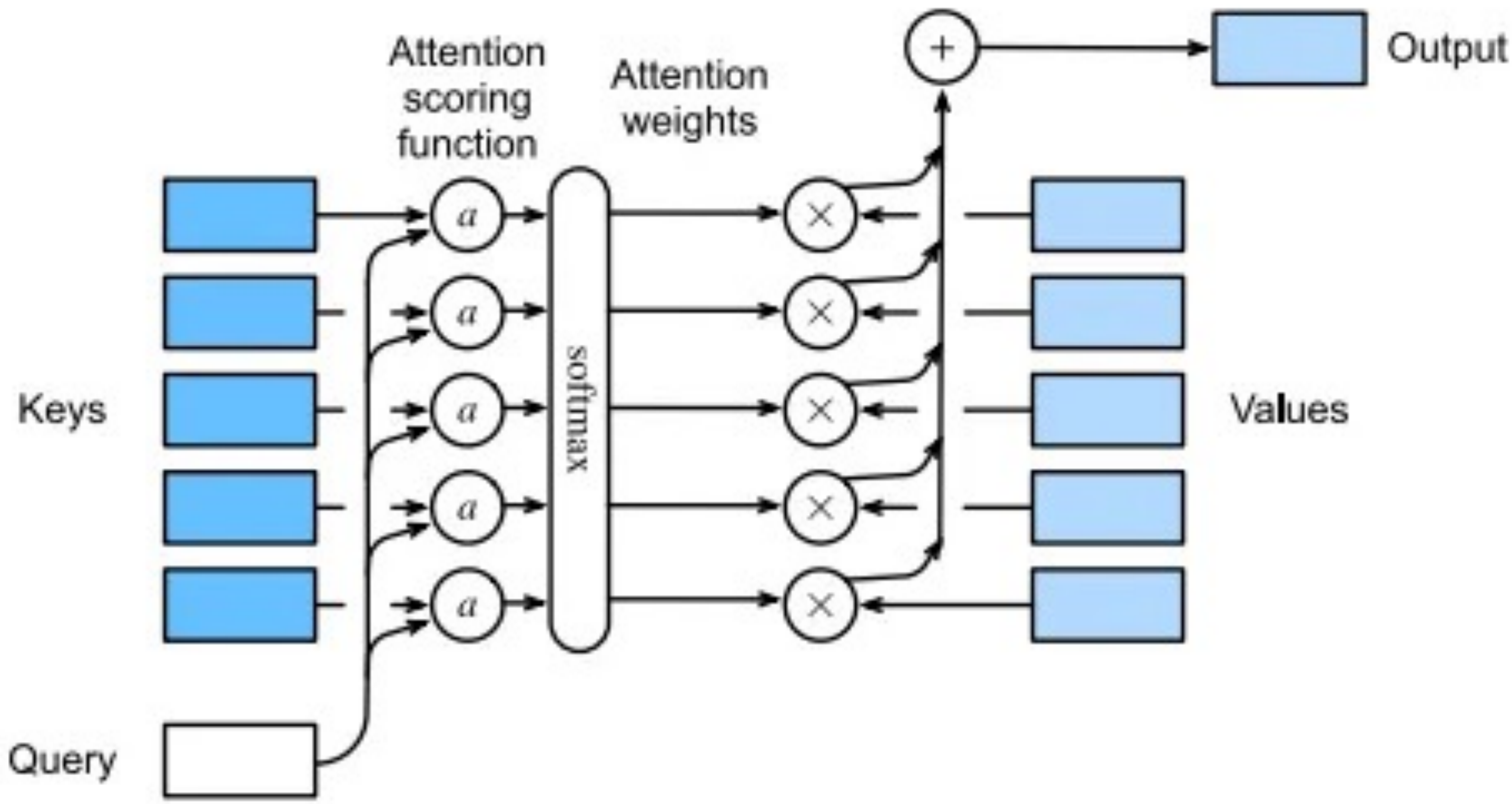


Attention Model

- Think about Queries, Keys, and Values
  - A Query describes what you're trying to do ("find the predator")
  - A Key describes a particular input ("red things")
  - A Value describes the value of that input ("one big red thing near the lower right")

Attention Model

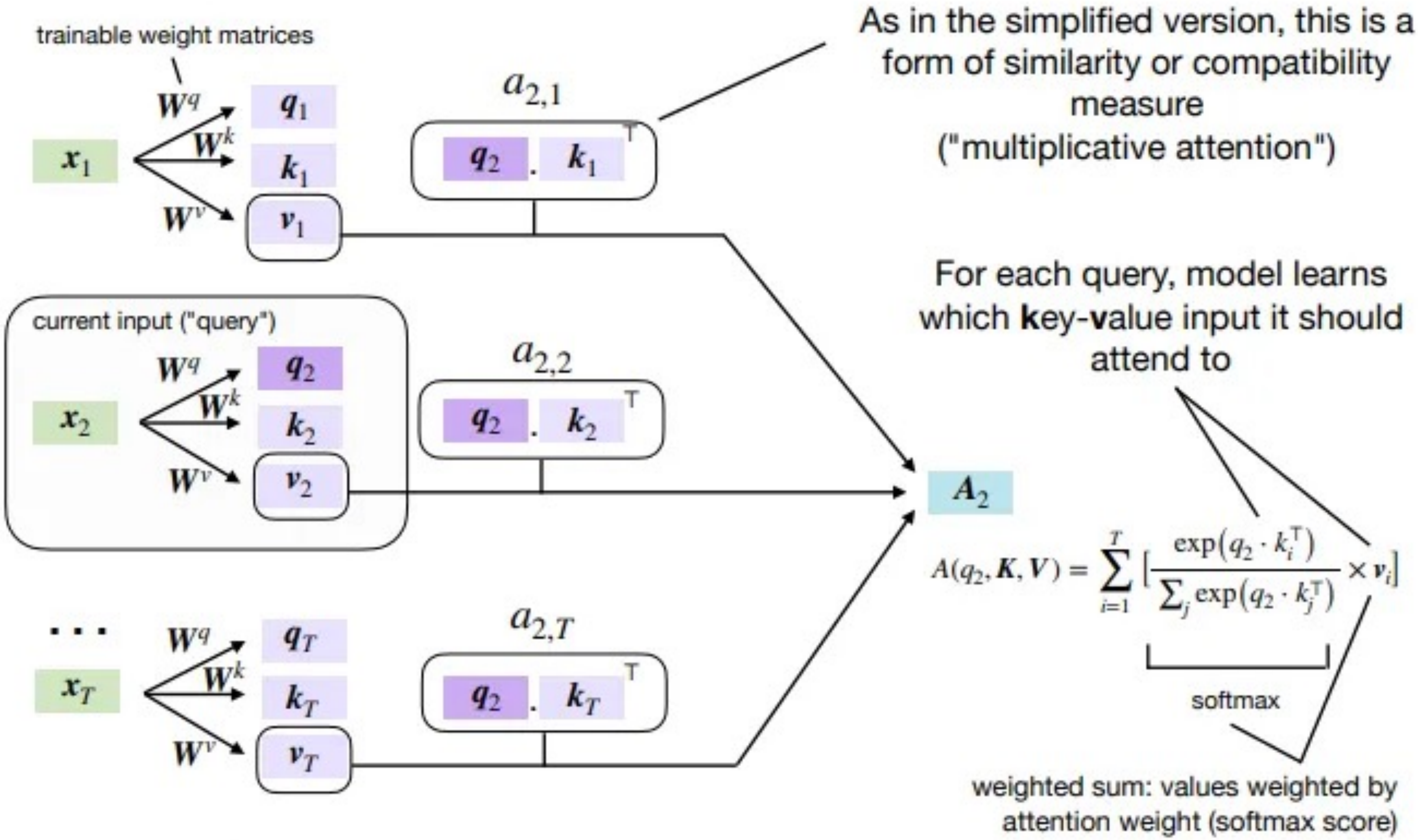


- Queries, Keys, and Values are vectors

Self-Attention

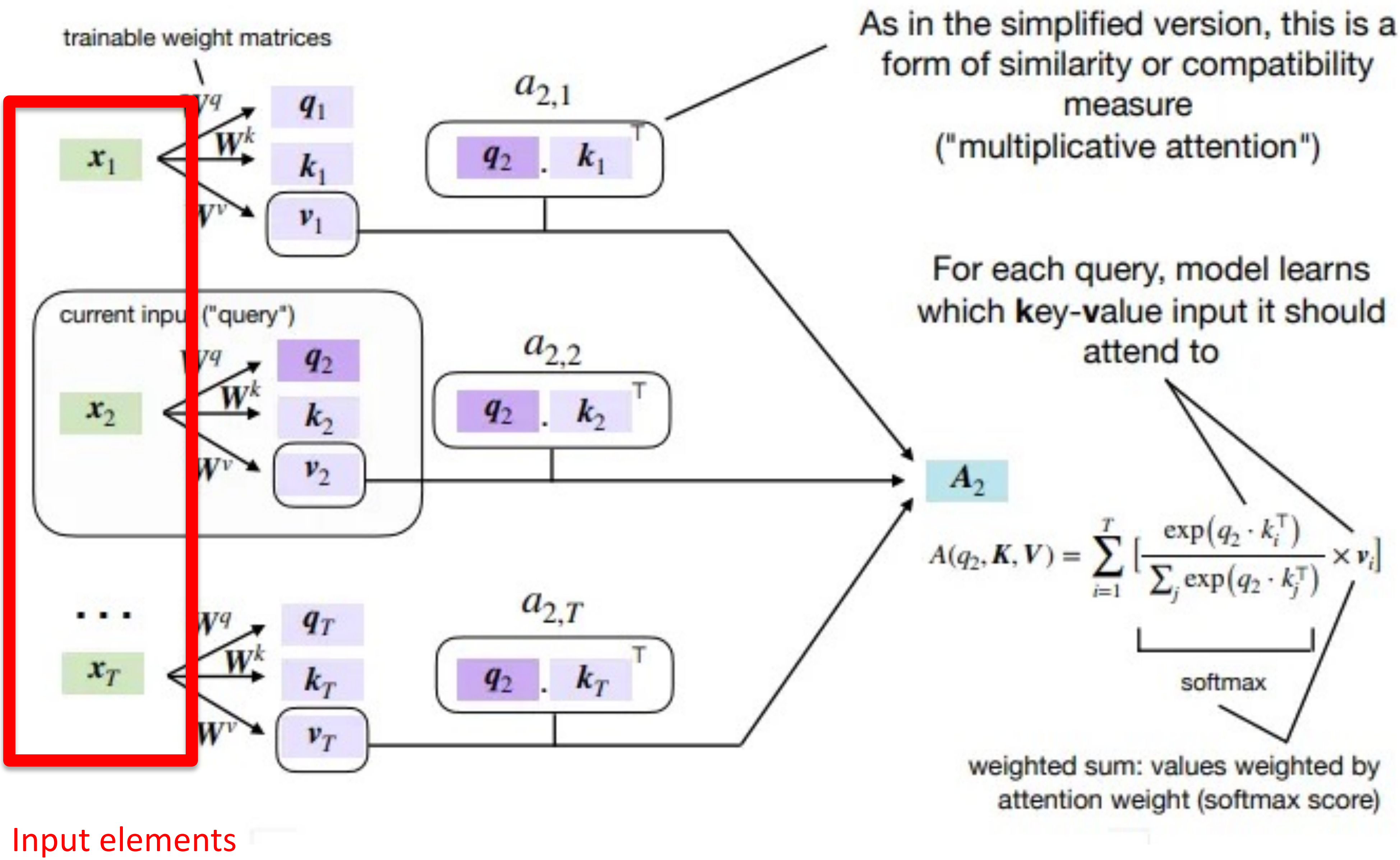
- Self-Attention works on an input sequence, allows us to drop the task-specific stuff
- We can encode both local and global dependencies

Self-Attention



Intro to Deep Learning by Sebastian Raschka

Self-Attention



Intro to Deep Learning by Sebastian Raschka

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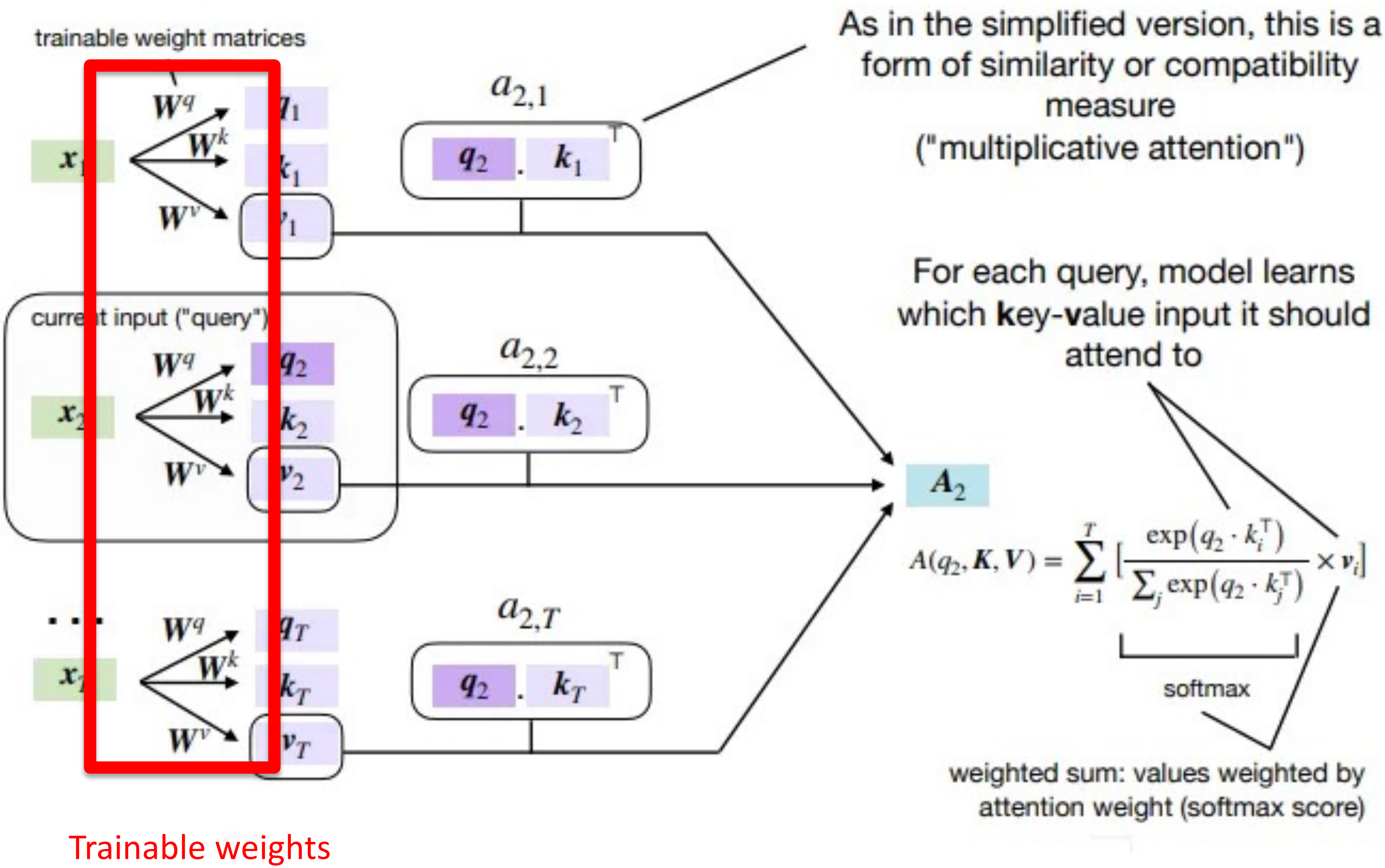
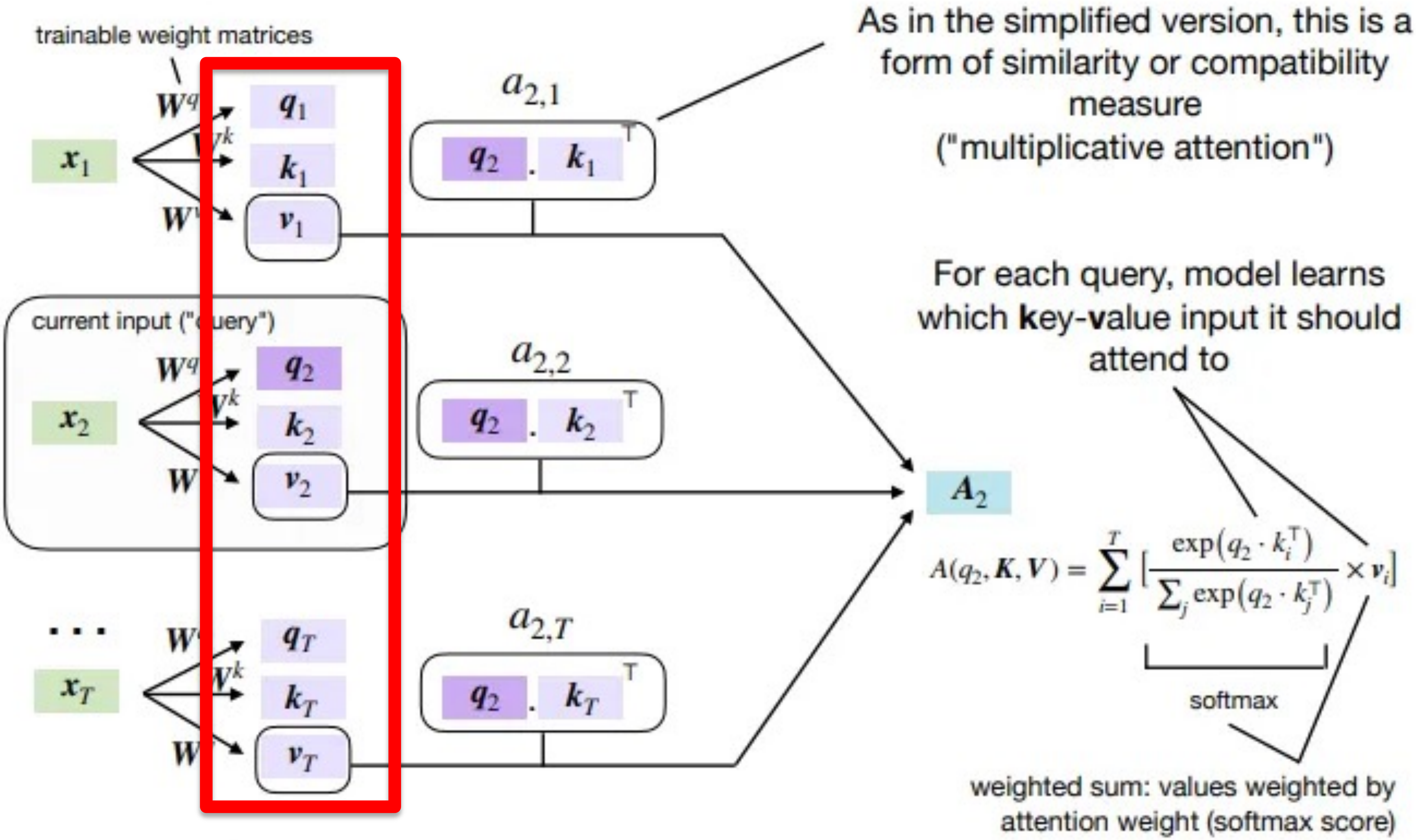


Intro to Deep Learning by Sebastian Raschka

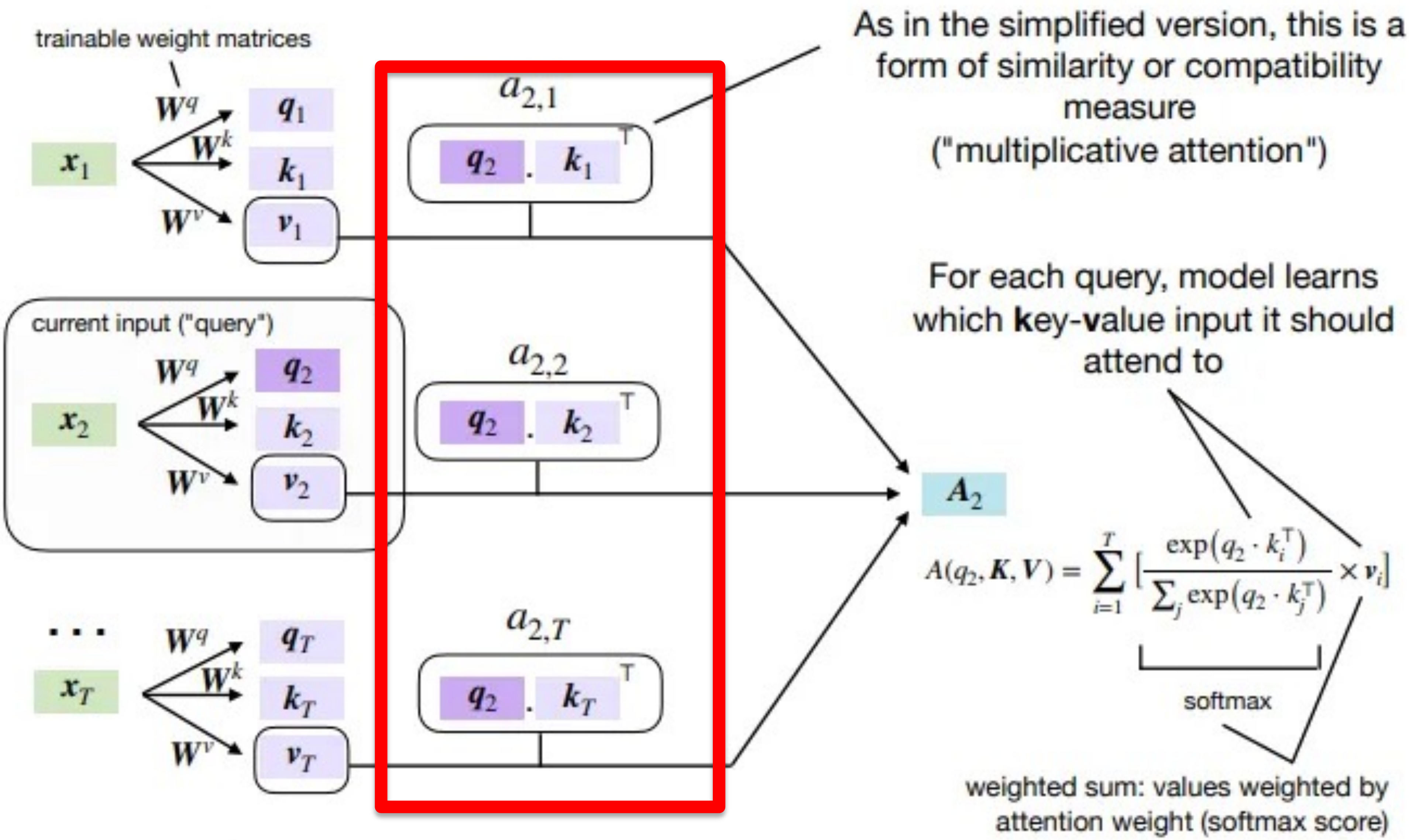
Self-Attention



Query, key, value vectors are result of combining input with learned weights

Intro to Deep Learning by Sebastian Raschka

Self-Attention

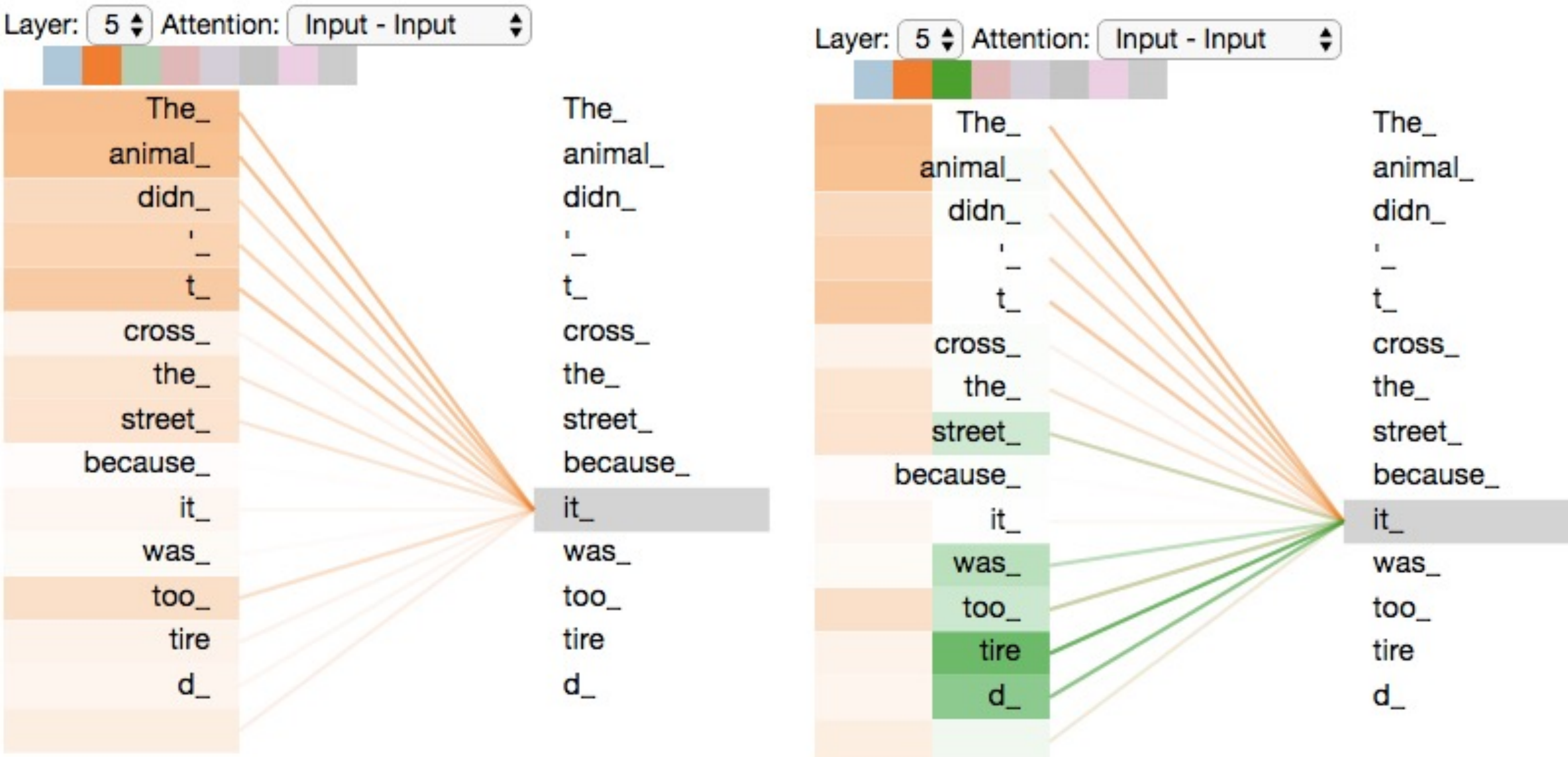


We combine q2 with each of the key$_i$ in order to obtain the attention we should pay to v$_i$ and we do this for all queries

Multi-Head Attention

- Compute the Self-Attention mechanism multiple times in parallel
- Using different sets of learned W^q, W^k, W^v weights for each head
- More heads let us capture different kinds of attention

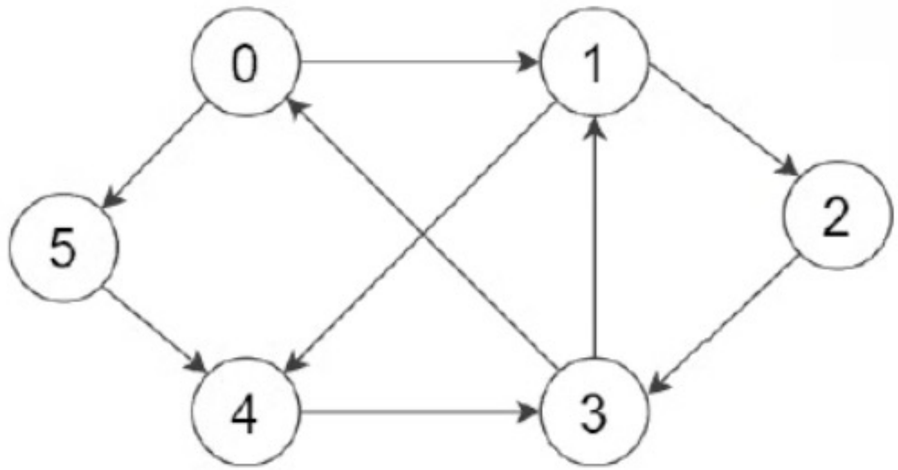
Multi-Head Attention



Allamar, The Illustrated Transformer

Karpathy's View of Attention

- Consider a directed graph, where each node stores a vector



- During "communication" nodes compute:
  - **Key vector**: What the node has
  - **Query vector**: What the node is looking for
  - **Value vector**: What the node will emit

Karpathy's View of Attention

- Encoder attention creates ”communication” or “message-passing” process
  - Loop over the nodes randomly
  - Each node combines its query vector with incoming nodes' key vectors; yields “interestingness” score of each input
  - Each node weights incoming values by score to yield an update to the node
- Attention in left-hand encoder “input” layer is fully connected, but masked MHA in decoder limits connectivity to reflect left-to-right text gen

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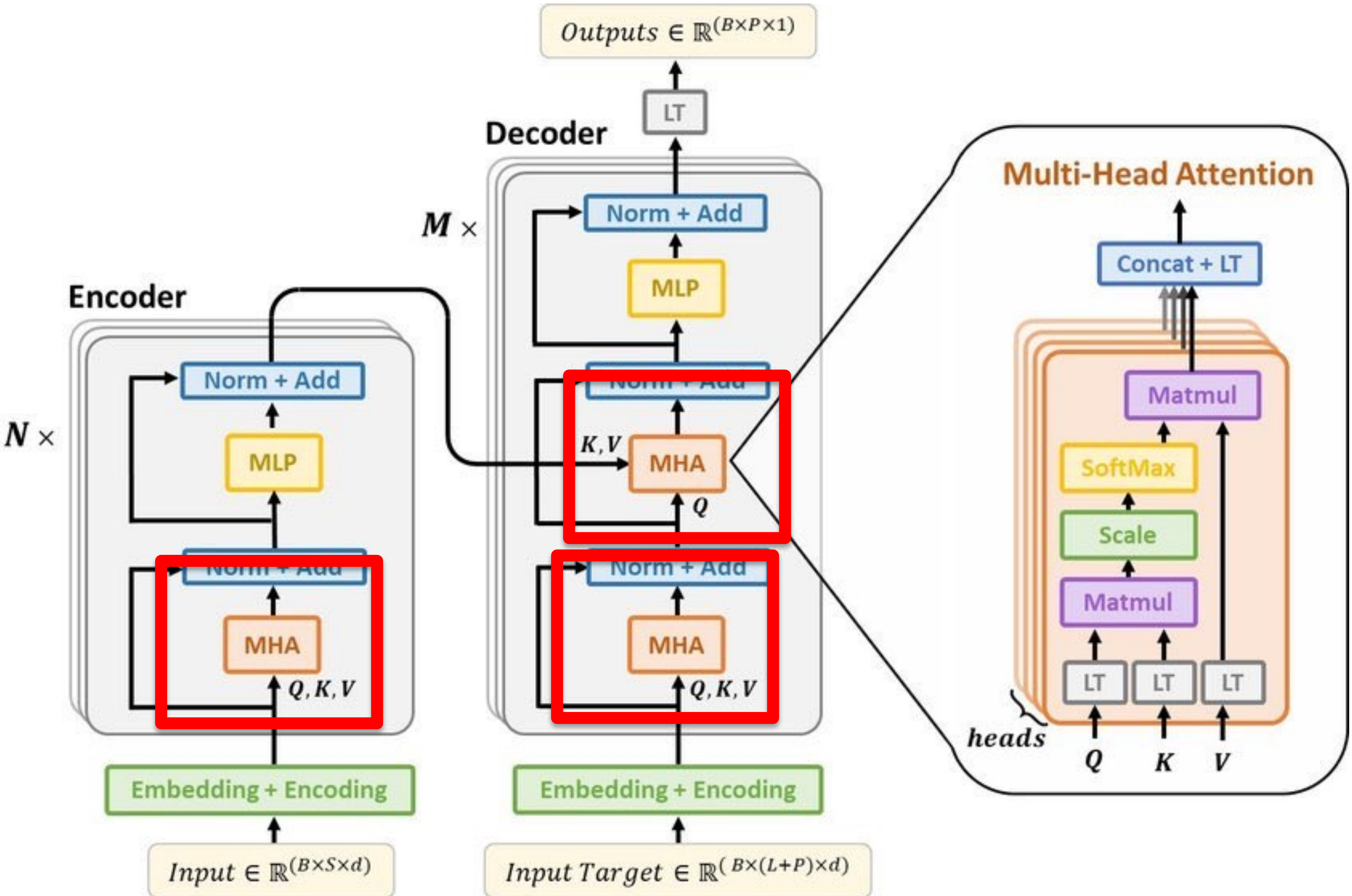
Transformers

- Most common architecture today is The Transformer
- “Attention is All You Need,” by Vaswani, Shazeer, Parmar, Uszkoreit, Jones, Gomez, Kaiser, Polosukhin (2017)
- Drops recurrence; eats entire input
- Still autoregressive

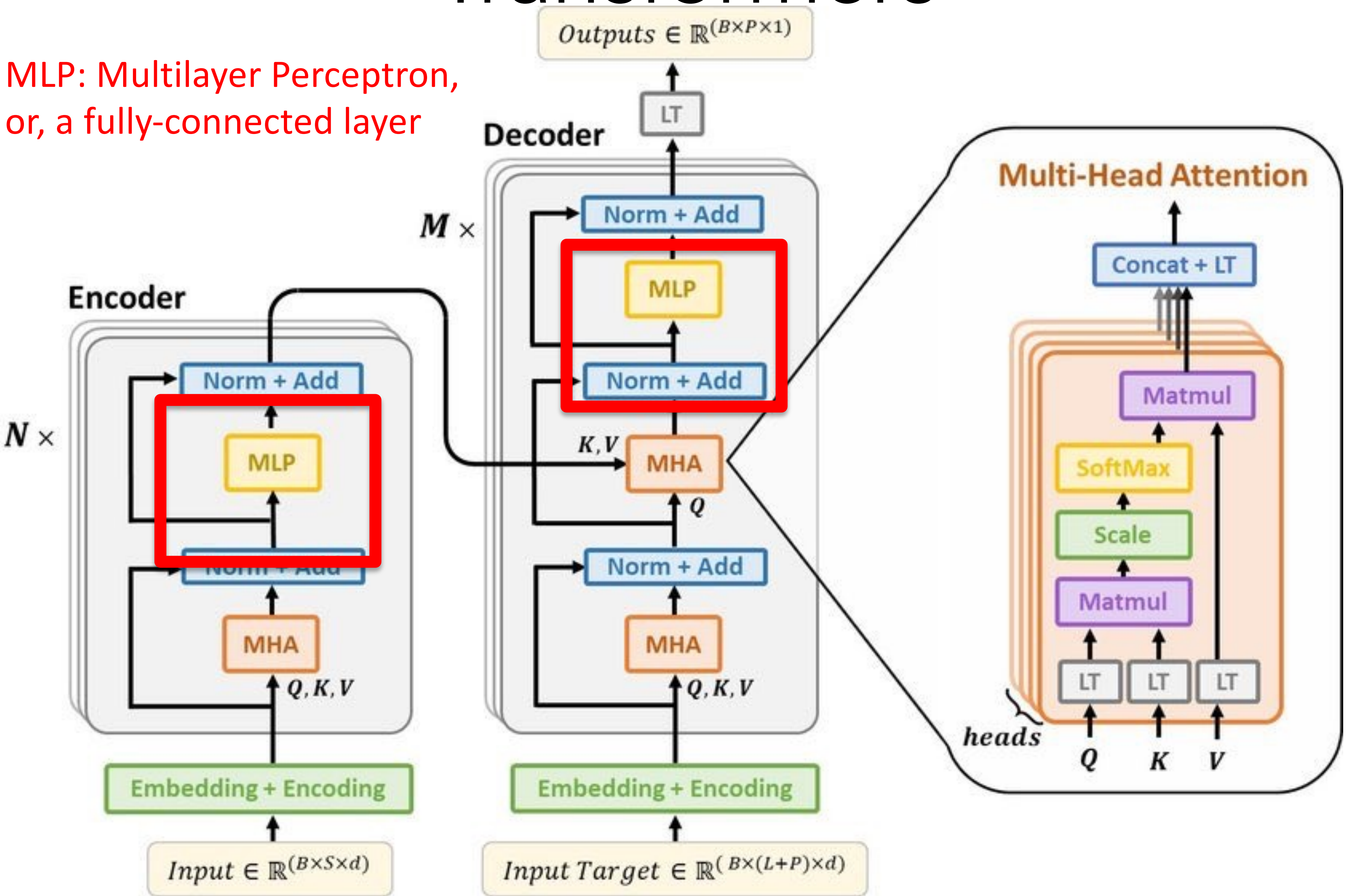
Transformers



https://www.researchgate.net/figure/The-Transformer-architecture-29-in-an-encoder-decoder-setting-adapted-to-facilitate_fig3_363085057

Transformers

MLP: Multilayer Perceptron,
or, a fully-connected layer

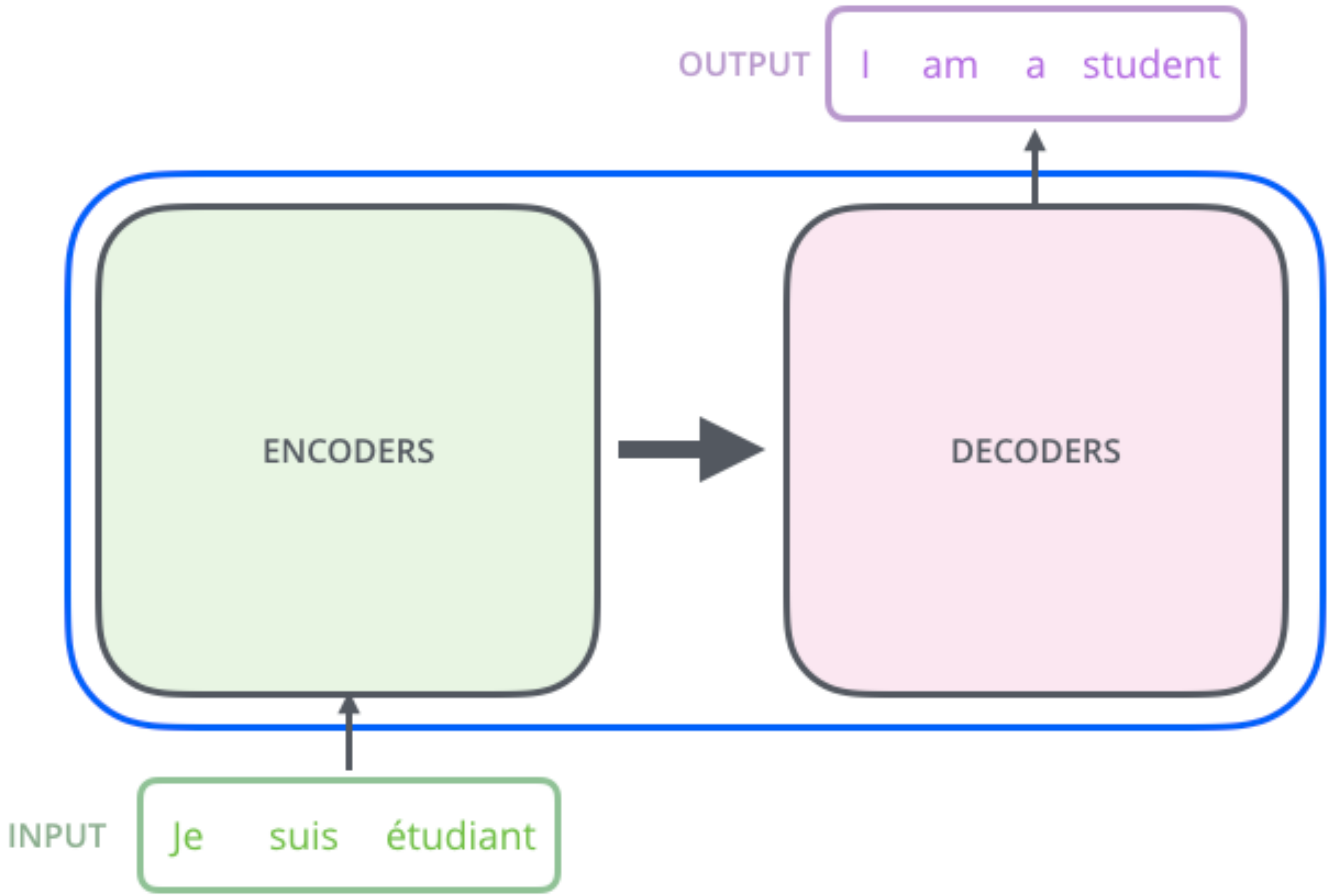


https://www.researchgate.net/figure/The-Transformer-architecture-29-in-an-encoder-decoder-setting-adapted-to-facilitate_fig3_363085057

Transformers

- Multi-Head attention is computed in parallel
- Each “pane” is replicated in series N times
- Different weights in each setting
- Masked MHA disallows attention to “future” tokens

Transformers



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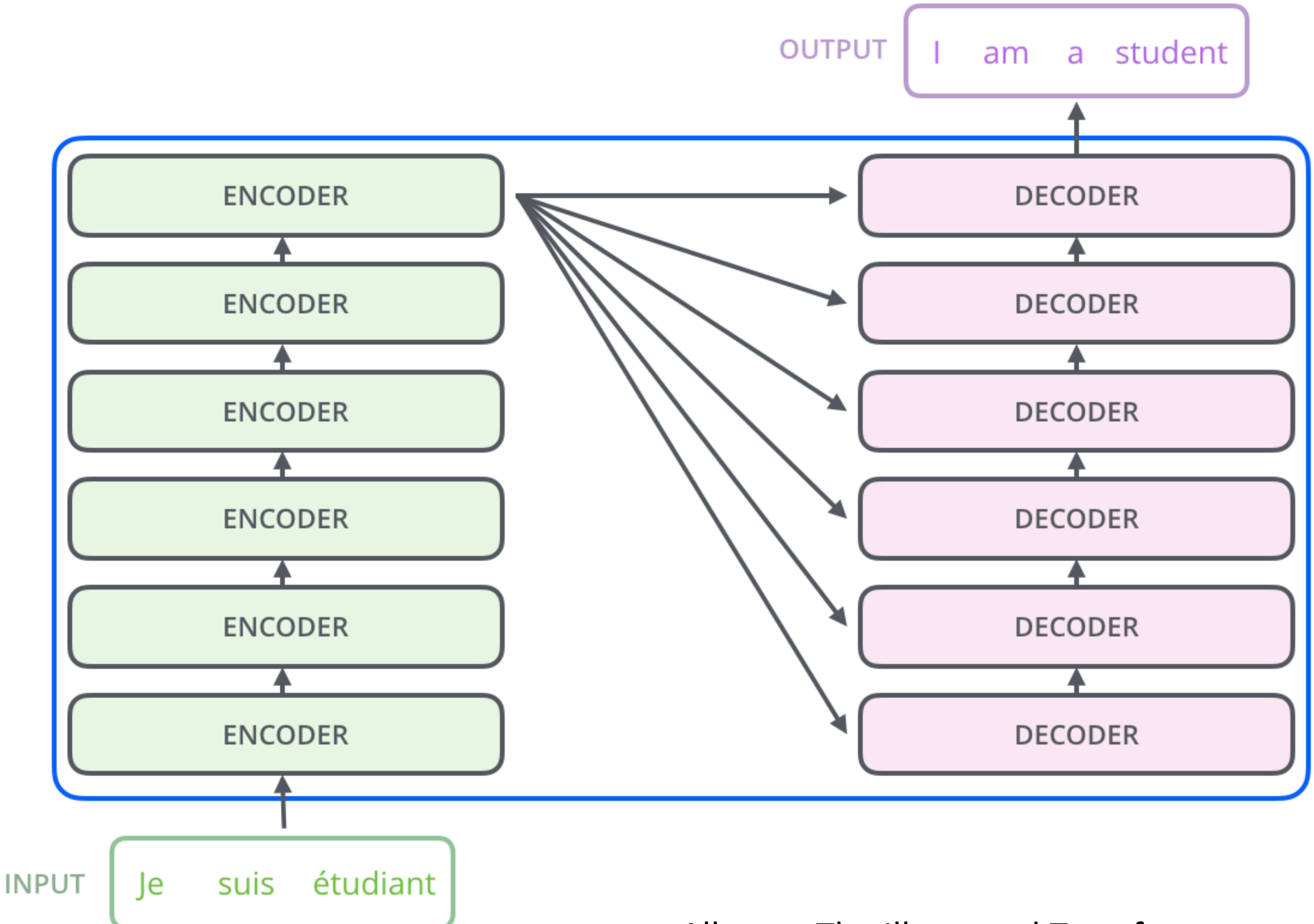
Transformers



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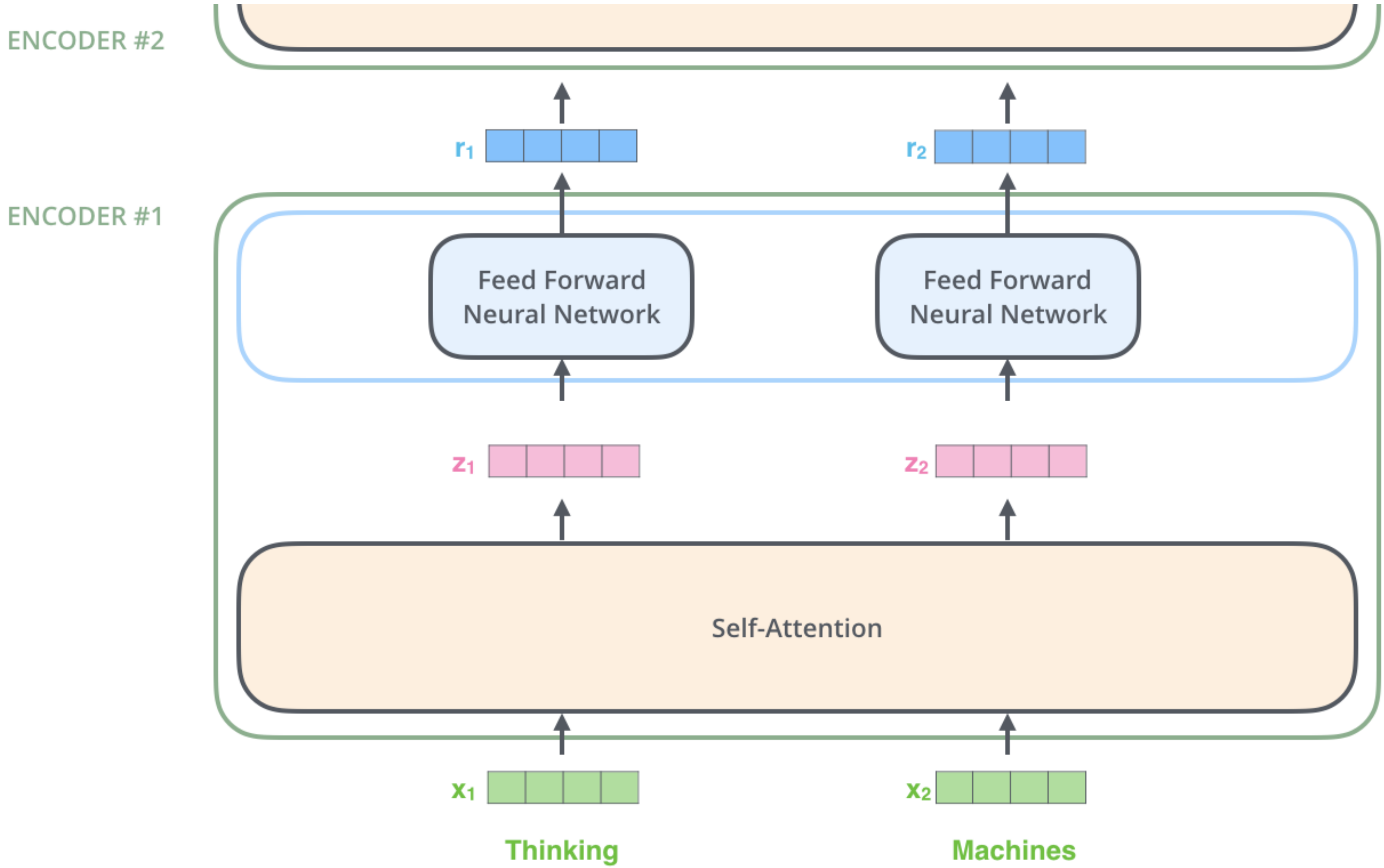

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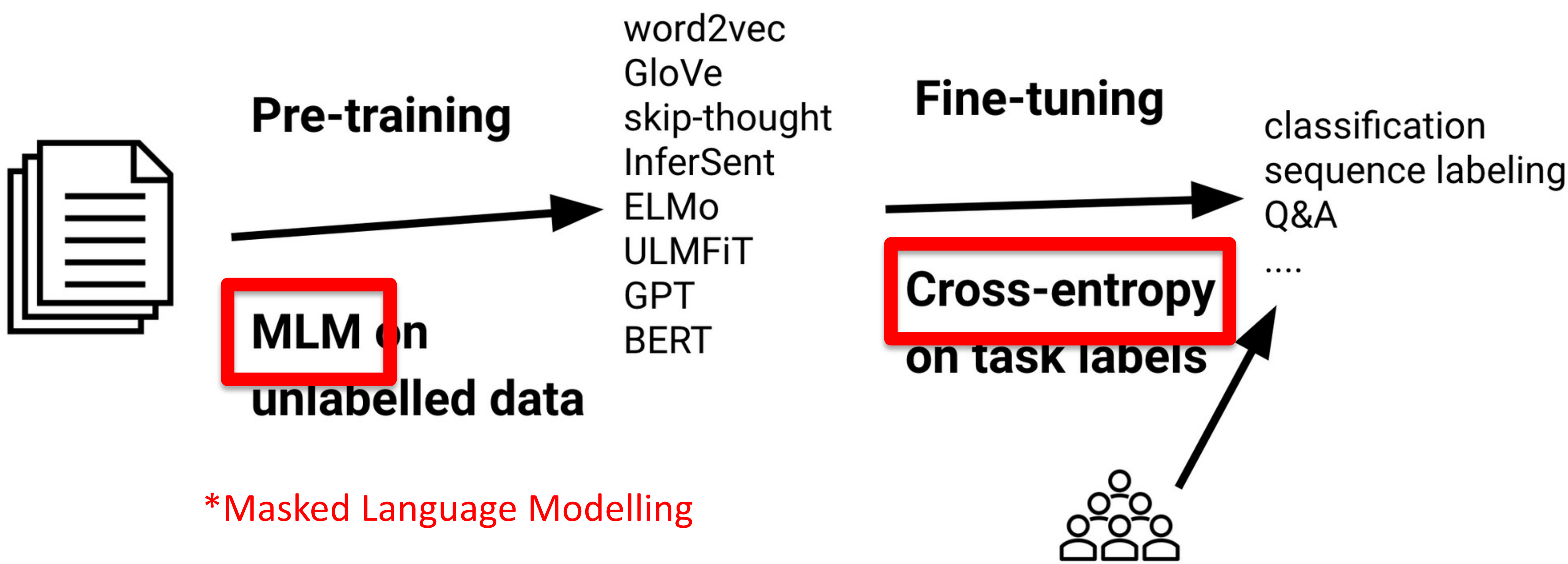
Putting It All Together

- We train a big language model, then fine-tune



*Masked Language Modelling

*Common loss function when training supervised learning model

- FT retrains, using small dataset & limited weight updates

Ruder, https://www.ruder.io/recent-advances-lm-fine-tuning/

Fine Tuning

- Fine-tuning allows us to adapt to a particular domain or particular task
- Often enables real improvements with relatively small training sets

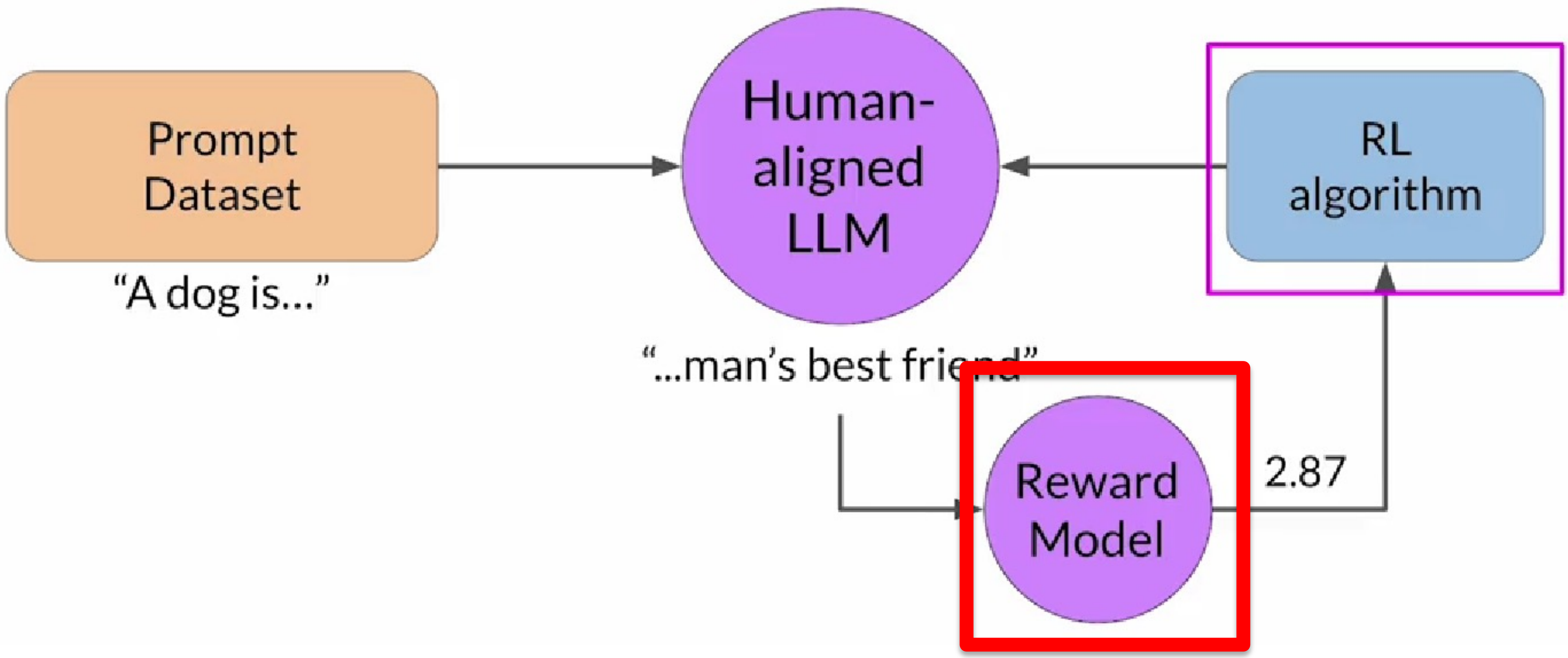
- **But,** what if we don’t have labeled data?
- **Also**, for a given output text, labeling it might be hard for a human, but choosing A vs B is easy

Reinforcement Learning with Human Feedback

- RLHF lets us use direct human feedback to fine-tune a model
- Often used to modify LLM tone, content guidelines, reducing “toxicity”

- Reinforcement Learning is AI area that uses “good dog/bad dog” signals instead of supervision

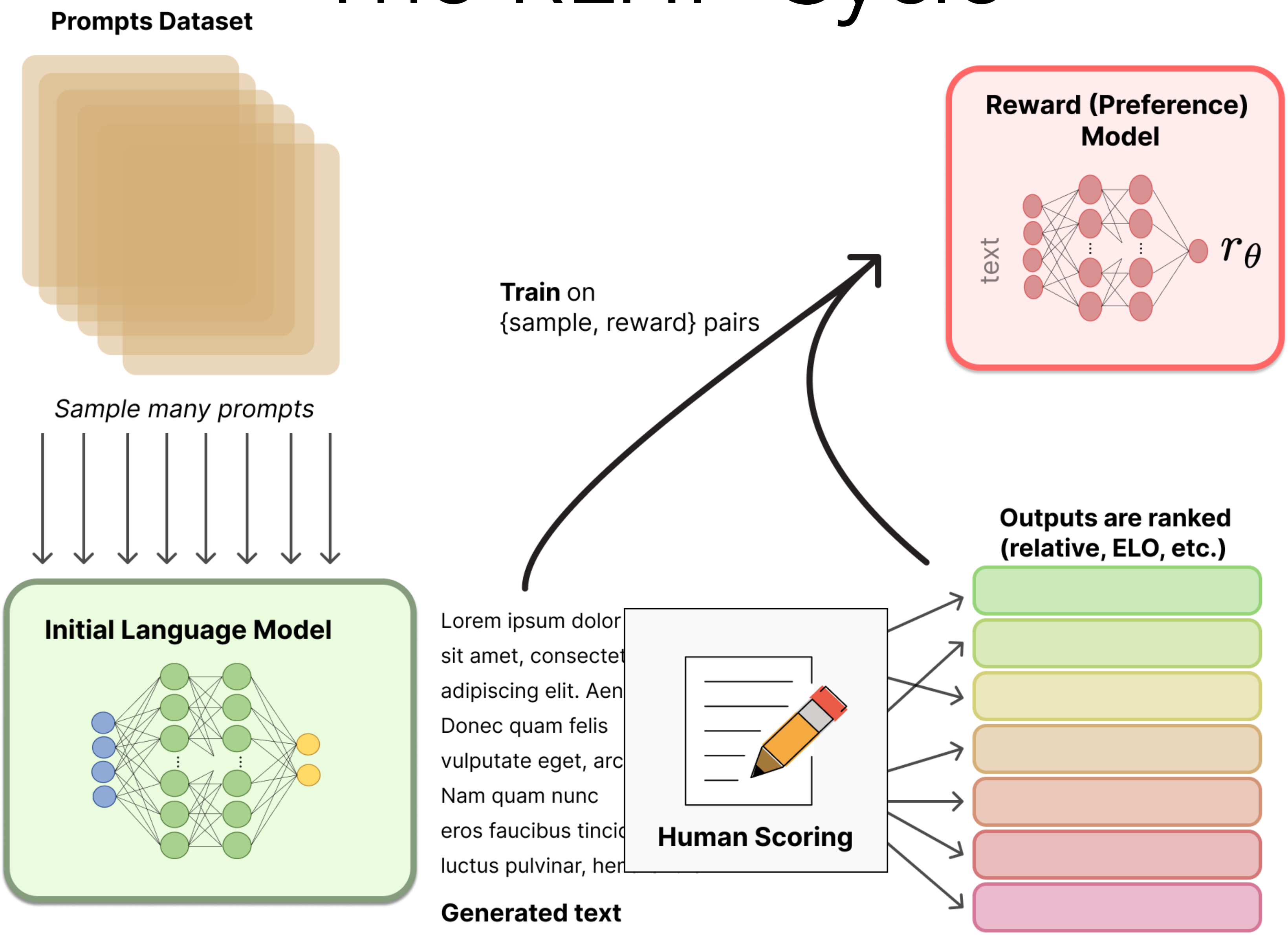
The RLHF Cycle



But how do we turn user preferences into a reward value?

https://www.ionio.ai/blog/a-comprehensive-guide-to-fine-tuning-llms-using-rlhf-part-1#reinforcement-learning-with-human-feedback-rlhf

The RLHF Cycle



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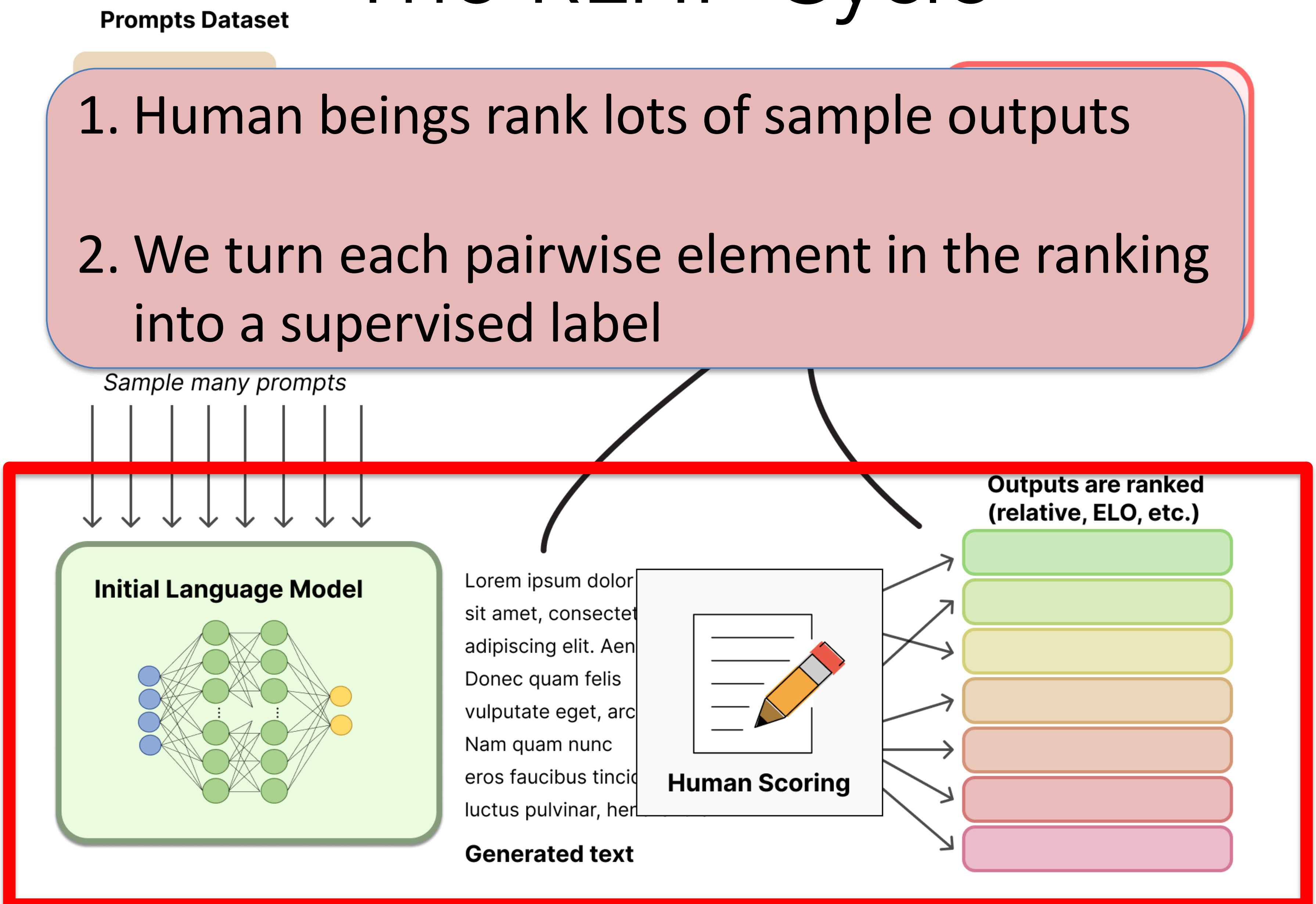
The RLHF Cycle

1. Human beings rank lots of sample outputs

2. We turn each pairwise element in the ranking into a supervised label



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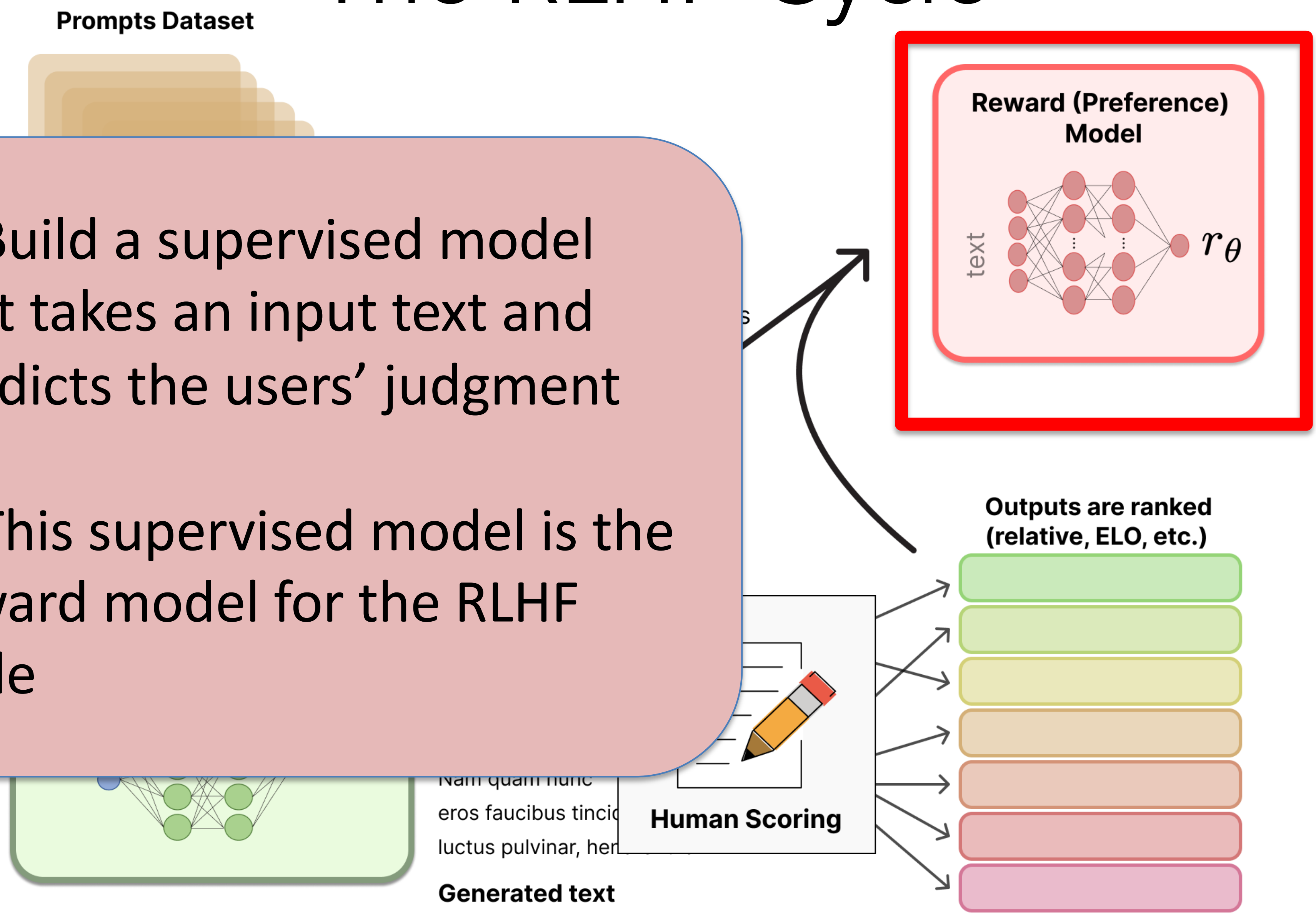
The RLHF Cycle

3. Build a supervised model that takes an input text and predicts the users' judgment

4. This supervised model is the reward model for the RLHF cycle



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RLHF Has Its Problems

- How much RL is too much? Hard to figure out when to stop
- Training the reward model is one place we can make mistakes, then fine-tuning adds another
- **Direct Preference Optimization** (Rafailov et al) is a new scheme that avoids constructing the reward model; part of Lab 5!