Natural Language Processing

Word2Vec to Transformer

Seongyun Lee

sy-lee@korea.ac.kr

Artificial Intelligence in KU (AIKU)

Department of Computer Science and Engineering, Korea University

AIKU

Contents

- **Week 4: Basic concepts of NLP from Word2Vec to Transformer**
- **Week 6: Diverse Transformer-family models and NLP tasks**

Representing words as discrete symbols

- In traditional NLP, we regard words as discrete symbols:
  - Hotel, conference, motel – a localist representation
    (one neuron represents one concepts)

Means one 1, the rest 0s

- Words can be represented by one-hot vectors:

motel = [0 0 0 0 0 0 0 0 0 0 1 0 0 0 0]

hotel = [0 0 0 0 0 0 0 1 0 0 0 0 0 0 0]

- Vector dimension = number of words in vocabulary (e.g. 500,000)

Representing words as discrete symbols

Example: in web search, if user searches for "Seattle motel", we would like to match documents containing "Seattle hotel" as well.

But:

motel = [0 0 0 0 0 0 0 0 0 0 1 0 0 0 0]

hotel = [0 0 0 0 0 0 0 1 0 0 0 0 0 0 0]

These two vectors are orthogonal - there is no natural notion of similarity for one-hot vectors!

Solution:

- Could try to rely on WordNet's list of synonyms to get similarity?
  - But it is well-known to fail badly: incompleteness, etc.
- **Instead: learn to encode similarity in the vectors themselves**

Word2Vec

- We will build a dense vector for each word, chosen so that it is similar to vectors of words that appear in similar contexts

$$\textit{banking} = \begin{pmatrix} 0.286 \\ 0.792 \\ -0.177 \\ -0.107 \\ 0.109 \\ -0.542 \\ 0.349 \\ 0.271 \end{pmatrix}$$

Note: word vectors are sometimes called word embeddings or word representations. They are a distributed representation.

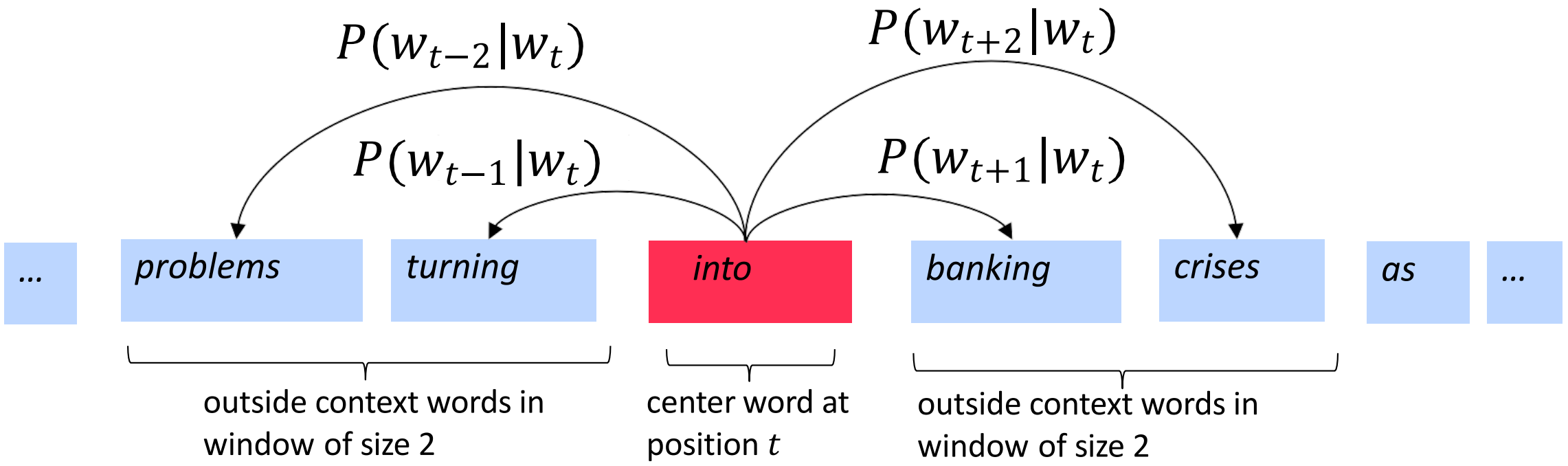
Word2Vec - Visualization

expect =

$$\begin{pmatrix} 0.286 \\ 0.792 \\ -0.177 \\ -0.107 \\ 0.109 \\ -0.542 \\ 0.349 \\ 0.271 \\ 0.487 \end{pmatrix}$$

Word2Vec - overview

- Example windows and process for computing $P(w_{t+j}|w_t)$



Word2Vec – objective function

- We want to minimize the objective function:

$$J(\theta) = -\frac{1}{T}\sum_{t=1}^{T}\sum_{\substack{-m\leq j\leq m \\ j\neq 0}} \log P\left(w_{t+j}\middle|w_t;\theta\right)$$

- **Question:** how to calculate $P\left(w_{t+j}\middle|w_t;\theta\right)$?
- **Answer:** we will use two vectors per word w:
  - v_w when w is a center word
  - u_w when w is a context word
- Then for a center word c and a context word o:

$$P(o|c) = \frac{\exp(u_o^\top v_c)}{\sum_{w\in V}\exp(u_w^\top v_c)}$$

Word2Vec – prediction function

2. Exponentiation makes anything positive

1. Dot product compares similarity of o and c.
$u^\top v = u \cdot v = \sum_{i=1}^{n} u_i v_i$
Larger dot product = larger probability

$$P(o|c) = \frac{\exp(u_o^\top v_c)}{\sum_{w \in V} \exp(u_w^\top v_c)}$$

3. Normalize over entire vocabulary to give probability distribution

- This is an example of the **softmax function** $\mathbb{R}^n \to (0,1)^n$ ← Open region

$$\text{softmax}(x_i) = \frac{\exp(x_i)}{\sum_{j=1}^{n} \exp(x_j)} = p_i$$

- The softmax function maps arbitrary values x_i to a probability distribution p_i
  - "max" because amplifies probability of largest x_i
  - "soft" because still assigns some probability to smaller x_i
  - Frequently used in Deep Learning

Intrinsic word vector evaluation

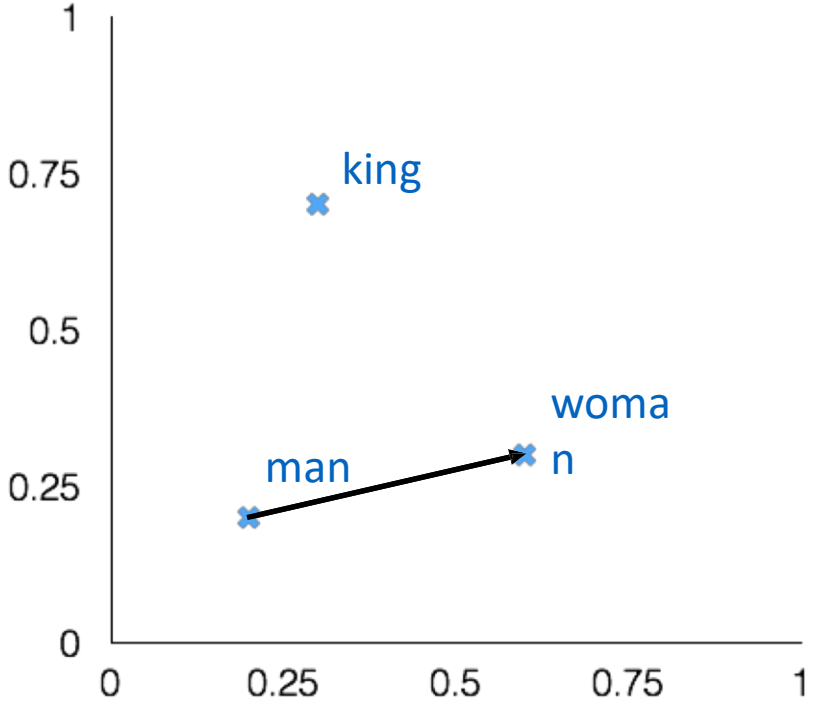
- Word vector analogies

a:b :: c:?

man:woman :: king:?

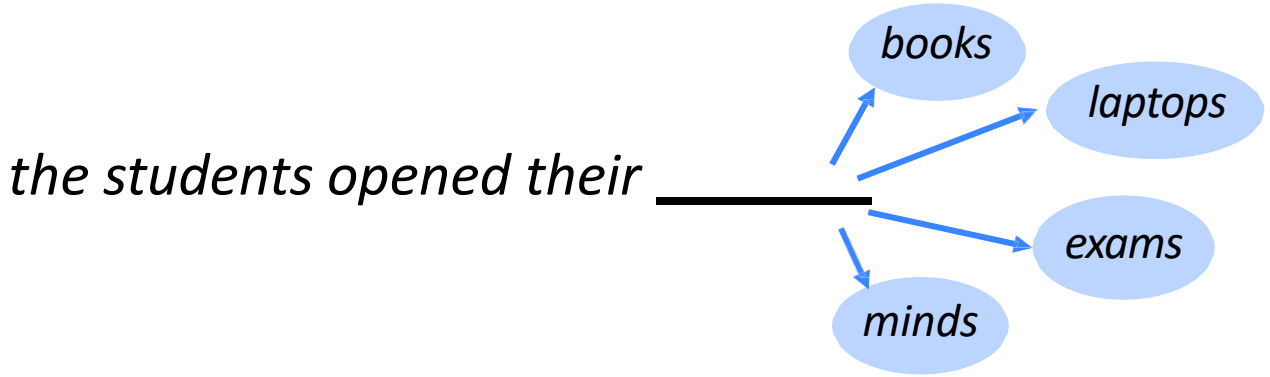
$$d = \arg\max_i \frac{(x_b - x_a + x_c)^T x_i}{||x_b - x_a + x_c||}$$

- Evaluate word vectors by how well their cosine distance after addition captures intuitive semantic and syntactic analogy questions
- Discarding the input words from the search!
- Problem: what if the information is there but not linear?



Language Modeling

- **Language Modeling** is the task of predicting what word comes next.



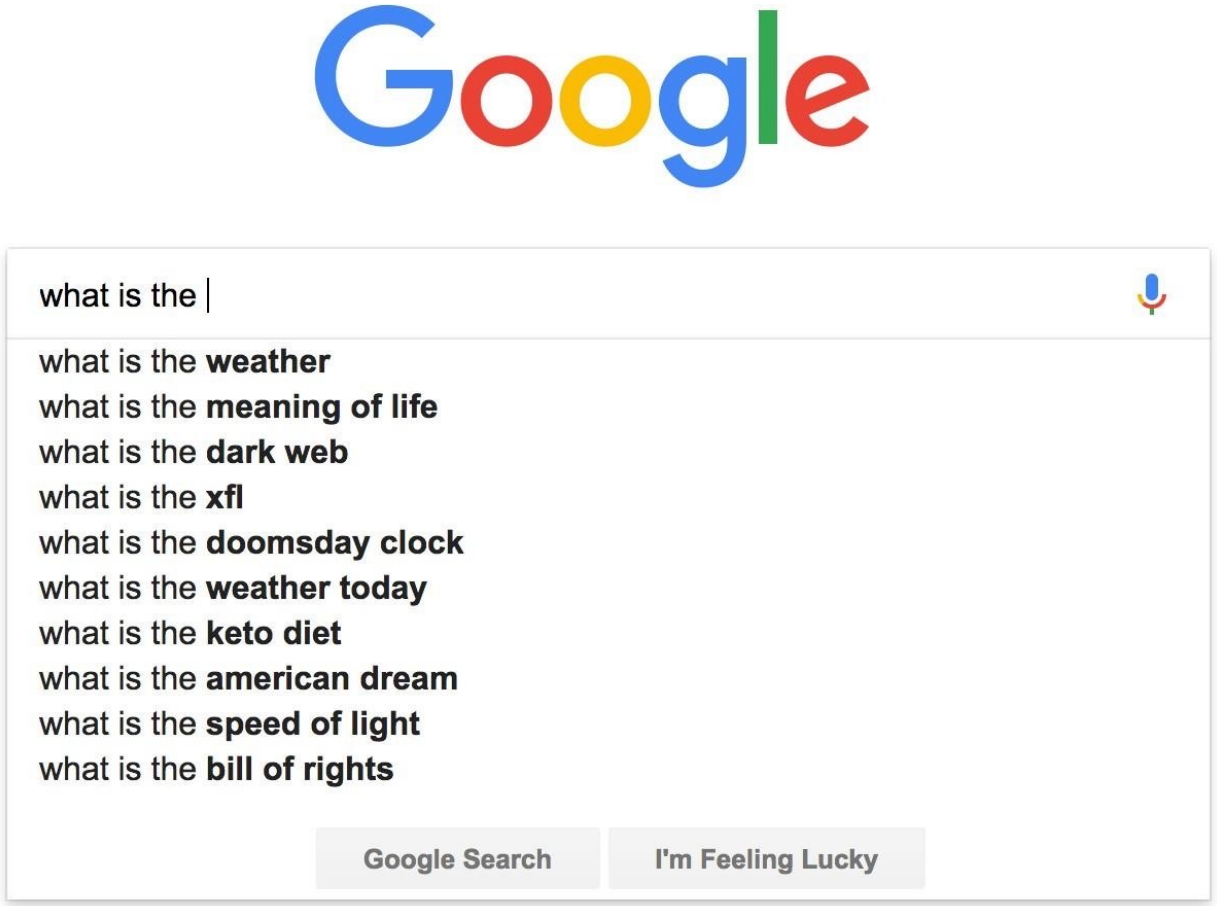
- More formally: given a sequence of words $\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}, \ldots, \boldsymbol{x}^{(t)}$, compute the probability distribution of the next word $\boldsymbol{x}^{(t+1)}$:

$$P(\boldsymbol{x}^{(t+1)} | \boldsymbol{x}^{(t)}, \ldots, \boldsymbol{x}^{(1)})$$

  where $\boldsymbol{x}^{(t+1)}$ can be any word in the vocabulary $V = \{\boldsymbol{w}_1, \ldots, \boldsymbol{w}_{|V|}\}$

- A system that does this is called a **Language Model**.

You use Language Models every day!



N-gram Language Models

the students opened their _____

- **Question**: How to learn a Language Model?
- **Answer** (pre- Deep Learning): learn a *n*-gram Language Model!

- Definition: A *n*-gram is a chunk of *n* consecutive words.
  - unigrams: “the”, “students”, “opened”, ”their”
  - bigrams: “the students”, “students opened”, “opened their”
  - trigrams: “the students opened”, “students opened their”
  - 4-grams: “the students opened their”

- Idea: Collect statistics about how frequent different n-grams are, and use these to predict next word.

Sparsity Problems with n-gram Language Models

Sparsity Problem 1

Problem: What if *"students opened their* $\boldsymbol{w}$*"* never occurred in data? Then $\boldsymbol{w}$ has probability 0!

(Partial) Solution: Add small δ to the count for every $\boldsymbol{w} \in V$. This is called *smoothing*.

$$P(\boldsymbol{w}|\text{students opened their}) = \frac{\text{count}(\text{students opened their } \boldsymbol{w})}{\text{count}(\text{students opened their})}$$

Sparsity Problem 2

Problem: What if *"students opened their"* never occurred in data? Then we can't calculate probability for *any* $\boldsymbol{w}$

(Partial) Solution: Just condition on *"opened their"* instead. This is called *backoff*.

Note: Increasing *n* makes sparsity problems *worse.* Typically we can't have *n* bigger than 5.

Generating text with a n-gram Language Model

- You can also use a Language Model to generate text.

today the price of gold per ton , while production of shoe l asts and shoe industry , the bank intervened just after it co nsidered and rejected an imf demand to rebuild depleted e uropean stocks , sept 30 end primary 76 cts a share .

Surprisingly grammatical!

…but **incoherent.** We need to consider more than three words at a time if we want to model language well.
But increasing *n* worsens sparsity problem,
and increases model size…

A fixed-window neural Language Model

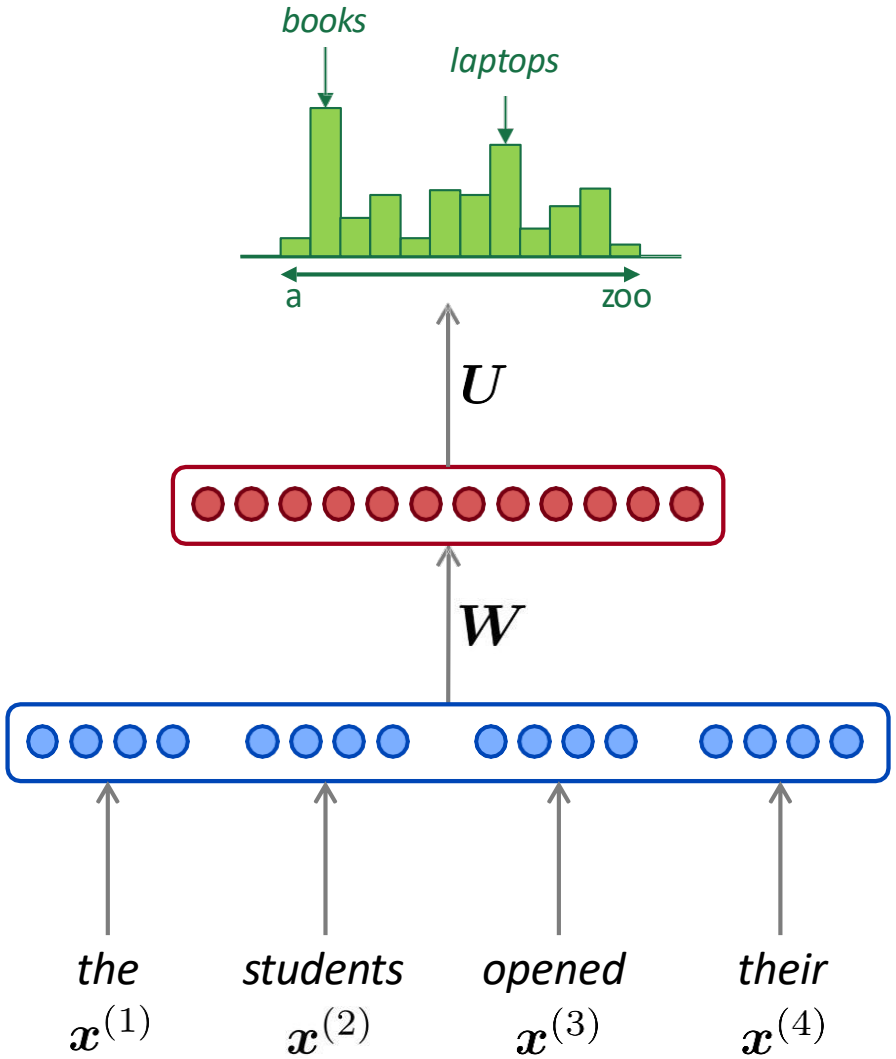
Improvements over *n*-gram LM:

- No sparsity problem
- Don't need to store all observed *n*-grams

Remaining **problems**:

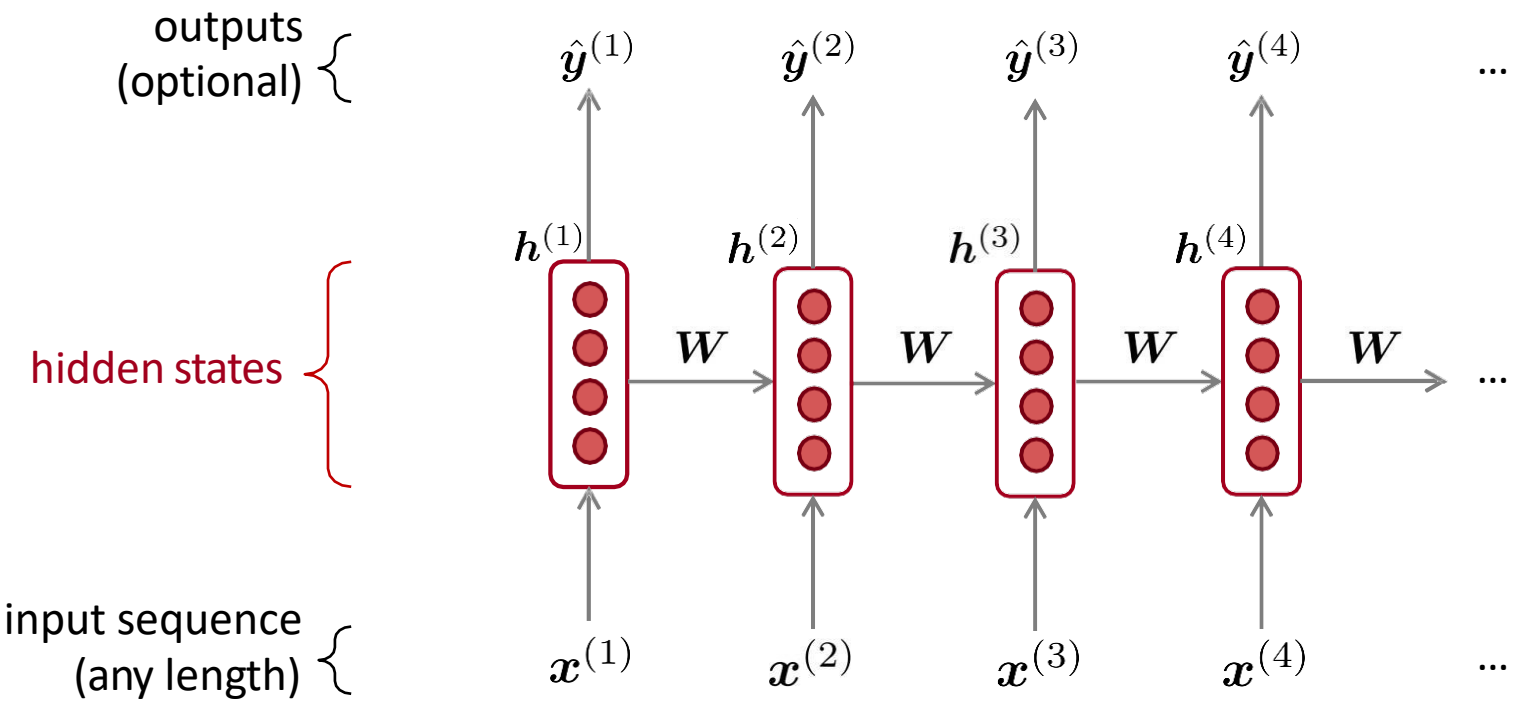
- Fixed window is too small
- Enlarging window enlarges $\boldsymbol{W}$
- Window can never be large enough!
- $\boldsymbol{x}^{(1)}$ and $\boldsymbol{x}^{(2)}$ are multiplied by completely different weights in $\boldsymbol{W}$. No symmetry in how the inputs are processed.

We need a neural architecture that can process *any length input*



Recurrent Neural Networks (RNN)

A family of neural architectures



Core idea: Apply the same weights W *repeatedly*

A RNN Language Model

$\hat{\boldsymbol{y}}^{(4)} = P(\boldsymbol{x}^{(5)}|\text{the students opened their})$

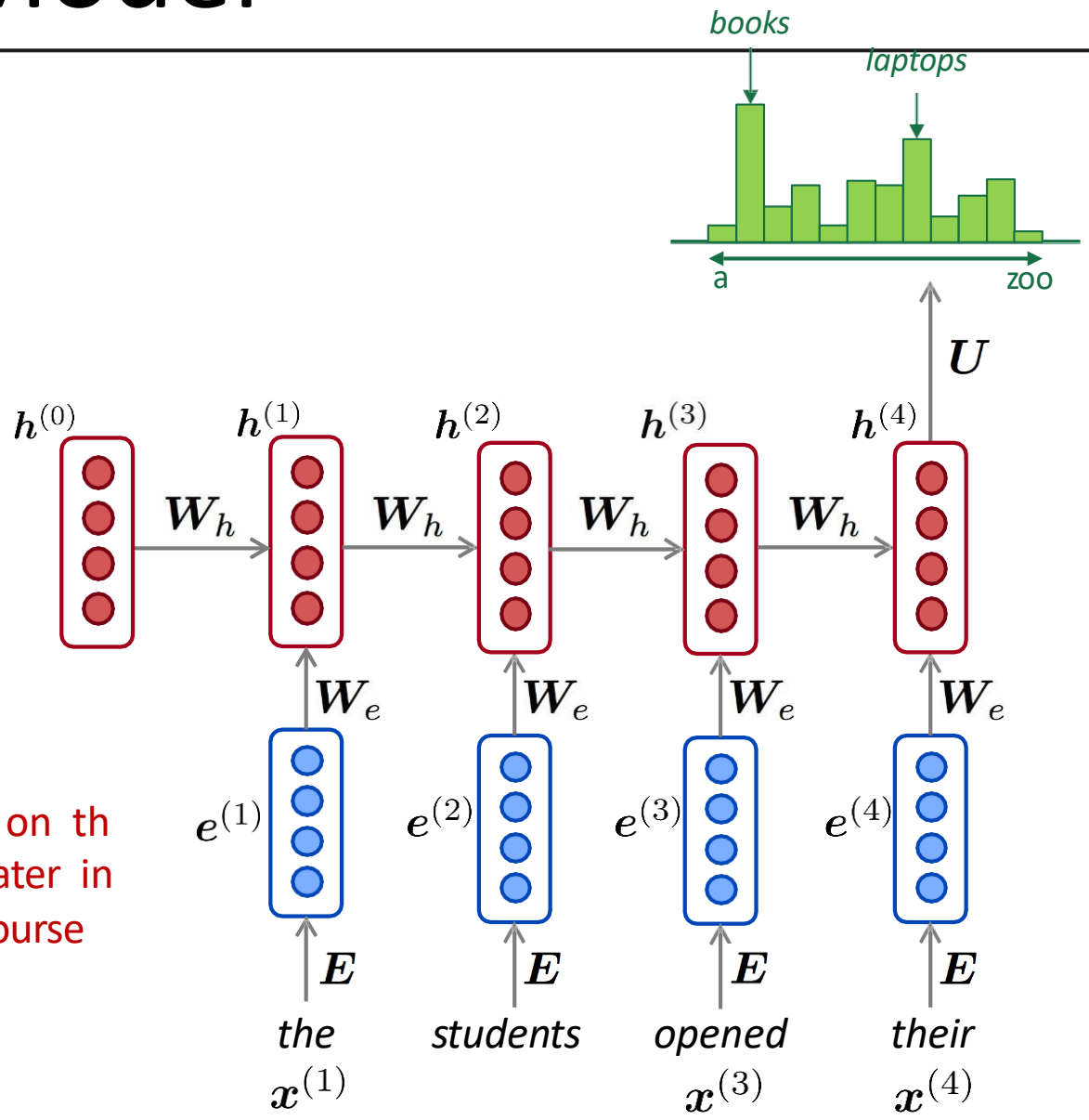
RNN **Advantages**:

- Can process any length input
- Computation for step *t* can (in theory) use information from many steps back
- Model size doesn't increase for longer input
- Same weights applied on every timestep, so there is symmetry in how inputs are processed.

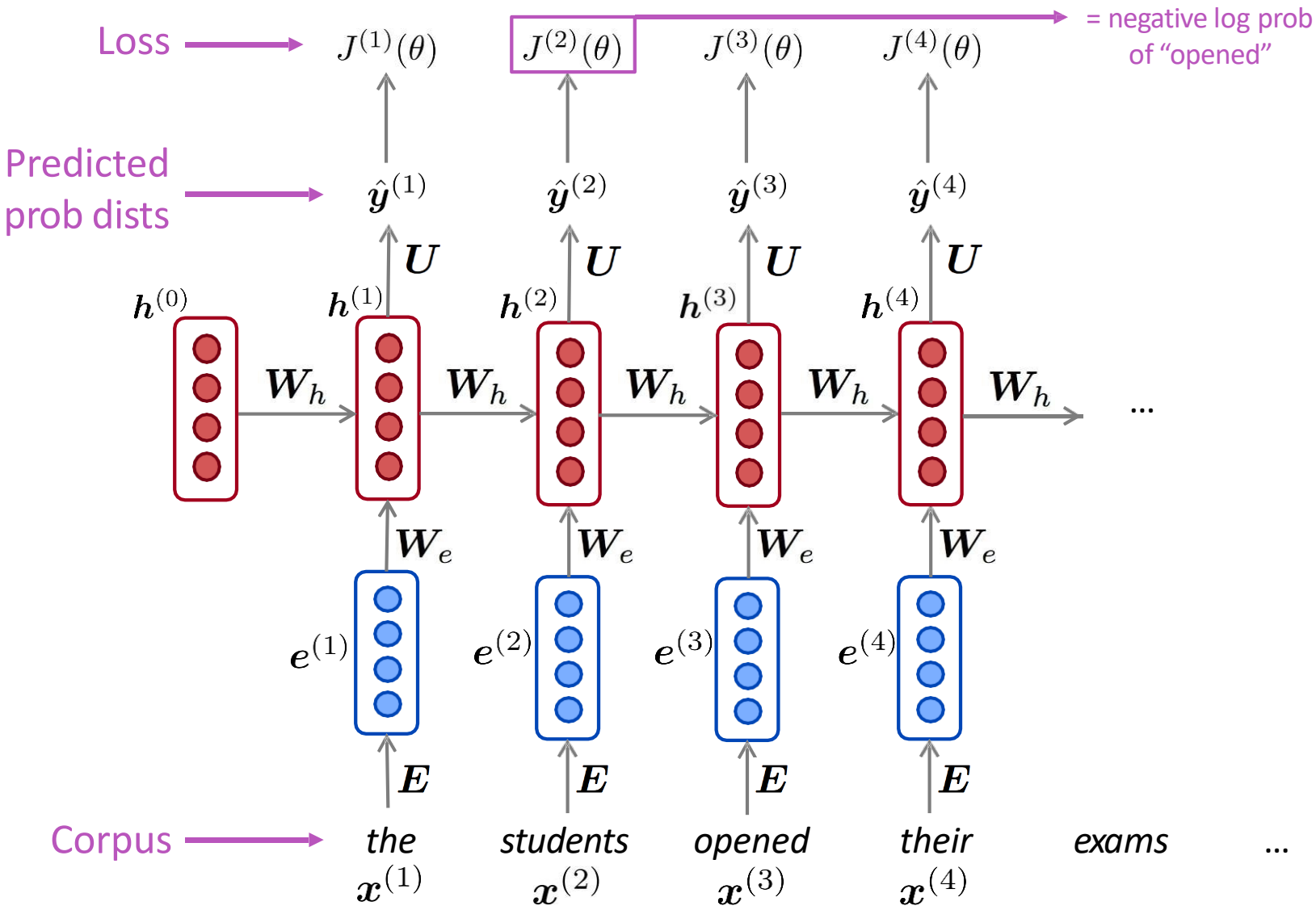
RNN **Disadvantages**:

- Recurrent computation is slow
- In practice, difficult to access information from many steps back

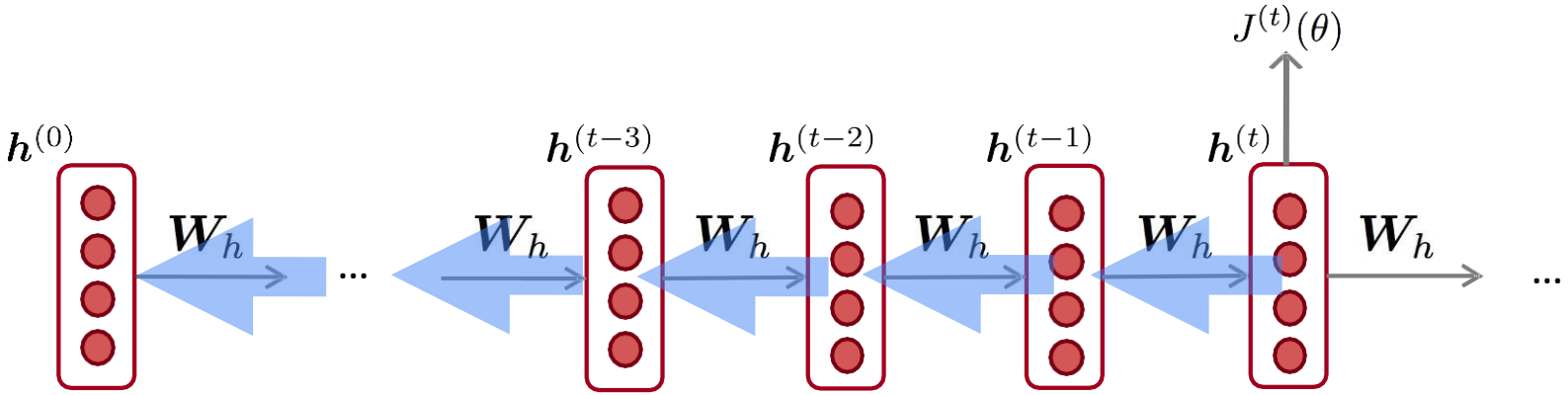
More on these later in the course



Training a RNN Language Model



Backpropagation for RNNs



$$\frac{\partial J^{(t)}}{\partial \boldsymbol{W_h}} = \sum_{i=1}^{t} \left. \frac{\partial J^{(t)}}{\partial \boldsymbol{W_h}} \right|_{(i)}$$

Question: How do we calculate this?

Answer: Backpropagate over timesteps *i*=*t*,…,0, summing gradients as you go.
This algorithm is called **"backpropagation through time"**

Generating text with a RNN Language Model

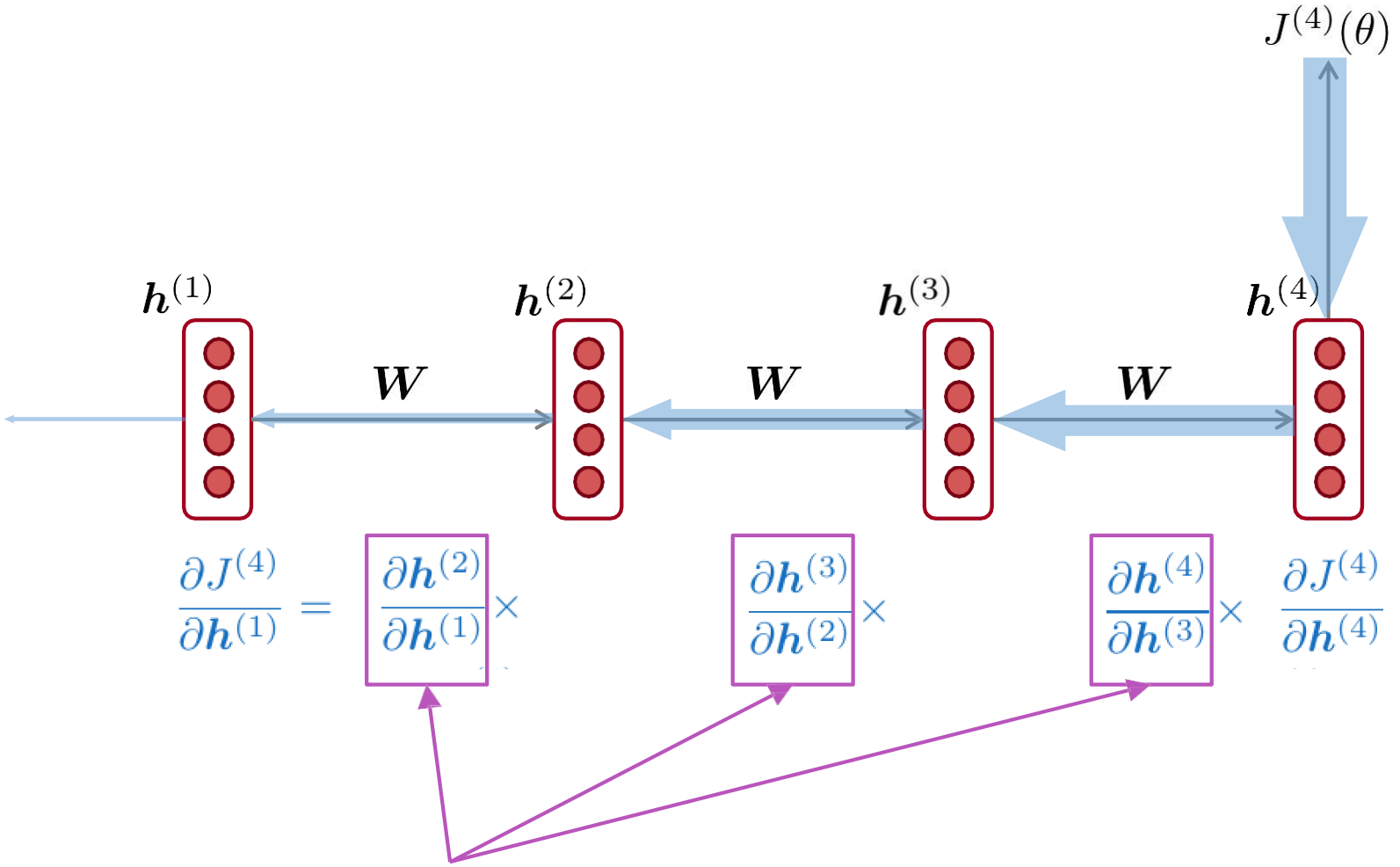
- Let's have some fun!
- You can train a RNN-LM on any kind of text, then generate text in that style.
- RNN-LM trained on *Harry Potter*:

"Sorry," Harry shouted, panicking—"I'll leave those brooms in London, are they?"

"No idea," said Nearly Headless Nick, casting low close by Cedric, carrying the last bit of treacle Charms, from Harry's shoulder, and to answer him the common room perched upon it, four arms held a shining knob from when the spider hadn't felt it seemed. He reached the teams too.

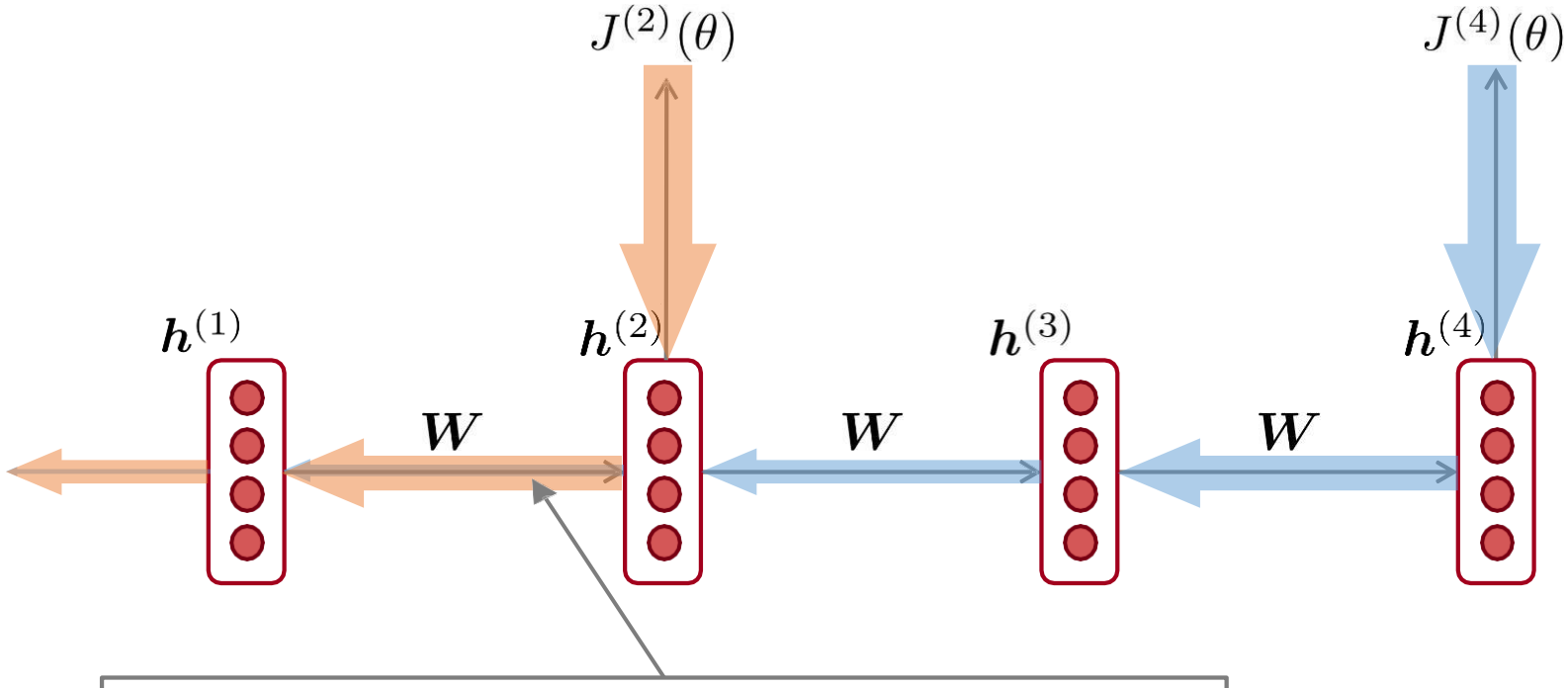
Source: https://medium.com/deep-writing/harry-potter-written-by-artificial-intelligence-8a9431803da6

Vanishing gradient intuition



Vanishing gradient problem:
When these are small, the gradient signal gets smaller and smaller as it backpropagates further

Why is vanishing gradient a problem?



Gradient signal from faraway is lost because it's much smaller than gradient signal from close-by.

So model weights are only updated only with respect to near effects, not long-term effects.

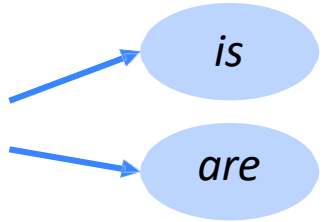
Why is vanishing gradient a problem?

- Another explanation: Gradient can be viewed as a measure of *the effect of the past on the future*

- If the gradient becomes vanishingly small over longer distances (step *t* to step *t+n*), then we can't tell whether:
  1. There's no dependency between step *t* and *t+n* in the data
  2. We have wrong parameters to capture the true dependency between *t* and *t+n*

Effect of vanishing gradient on RNN-LM

- **LM task:** *The writer of the books* ____



- **Correct answer**: *The writer of the books <u>is</u> planning a sequel*
- **Syntactic recency:** *The <u>writer</u> of the books <u>is</u>* (correct)
- **Sequential recency:** *The writer of the <u>books</u> <u>are</u>* (incorrect)
- Due to vanishing gradient, RNN-LMs are better at learning from sequential recency than syntactic recency, so they make this typ e of error more often than we'd like [Linzen et al 2016]

Long Short-Term Memory (LSTM)

We have a sequence of inputs $\boldsymbol{x}^{(t)}$, and we will compute a sequence of hidden states $\boldsymbol{h}^{(t)}$ and cell states $\boldsymbol{c}^{(t)}$.

On timestep *t*:

Forget gate: controls what is kept vs forgotten, from previous cell state

Input gate: controls what parts of the new cell content are written to cell

Output gate: controls what parts of cell are output to hidden state

New cell content: this is the new content to be written to the cell

Cell state: erase ("forget") some content from last cell state, and write ("input") some new cell content

Hidden state: read ("output") some content from the cell

Sigmoid function: all gate values are between 0 and 1

$$\boldsymbol{f}^{(t)} = \sigma\left(\boldsymbol{W}_f\boldsymbol{h}^{(t-1)} + \boldsymbol{U}_f\boldsymbol{x}^{(t)} + \boldsymbol{b}_f\right)$$

$$\boldsymbol{i}^{(t)} = \sigma\left(\boldsymbol{W}_i\boldsymbol{h}^{(t-1)} + \boldsymbol{U}_i\boldsymbol{x}^{(t)} + \boldsymbol{b}_i\right)$$

$$\boldsymbol{o}^{(t)} = \sigma\left(\boldsymbol{W}_o\boldsymbol{h}^{(t-1)} + \boldsymbol{U}_o\boldsymbol{x}^{(t)} + \boldsymbol{b}_o\right)$$

$$\tilde{\boldsymbol{c}}^{(t)} = \tanh\left(\boldsymbol{W}_c\boldsymbol{h}^{(t-1)} + \boldsymbol{U}_c\boldsymbol{x}^{(t)} + \boldsymbol{b}_c\right)$$

$$\boldsymbol{c}^{(t)} = \boldsymbol{f}^{(t)} \circ \boldsymbol{c}^{(t-1)} + \boldsymbol{i}^{(t)} \circ \tilde{\boldsymbol{c}}^{(t)}$$

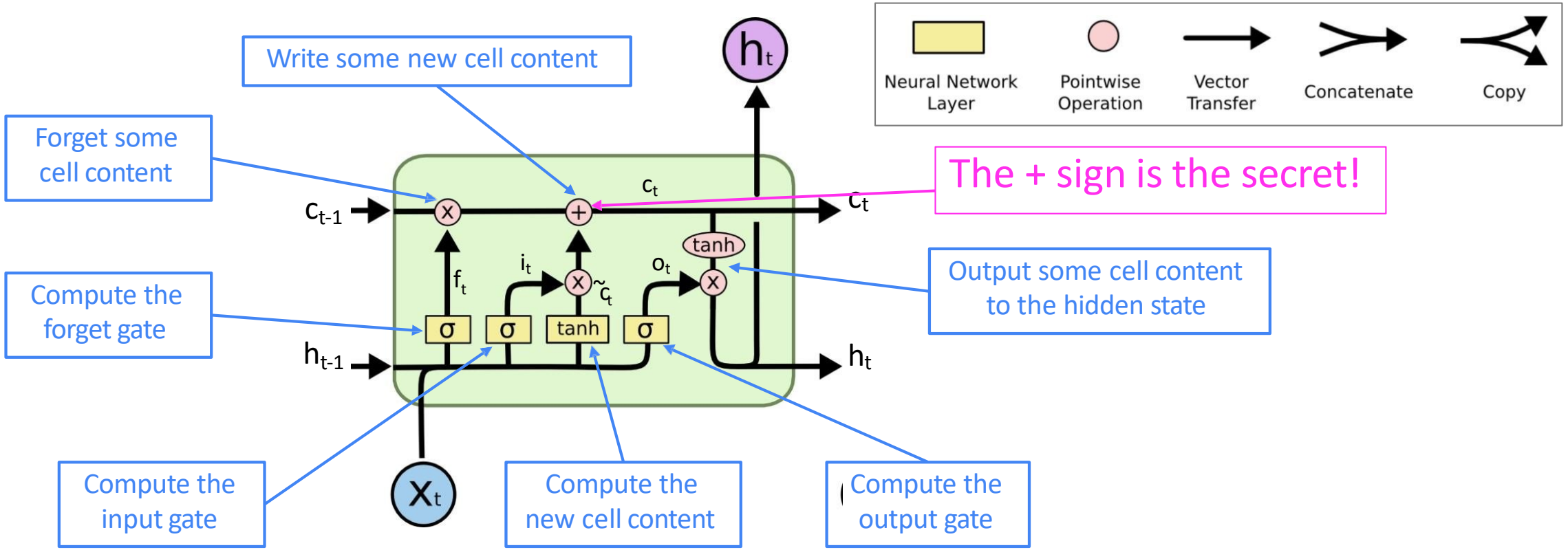
$$\boldsymbol{h}^{(t)} = \boldsymbol{o}^{(t)} \circ \tanh \boldsymbol{c}^{(t)}$$

Gates are applied using element-wise product

All these are vectors of same length *n*

Long Short-Term Memory (LSTM)

You can think of the LSTM equations visually like this:



How does LSTM solve vanishing gradients?

- The LSTM architecture makes it easier for the RNN to preserve information over many timesteps
  - e.g. if the forget gate is set to remember everything on every timestep, then the info in the cell is preserved indefinitely
  - By contrast, it's harder for vanilla RNN to learn a recurrent weight matrix W_h that preserves info in hidden state
  - In practice, you get about 100 timesteps rather than about 7

- LSTM doesn't *guarantee* that there is no vanishing/exploding gradient, but it does provide an easier way for the model to l earn long-distance dependencies

Gated Recurrent Units (GRU)

- Proposed by Cho et al. in 2014 as a simpler alternative to the LSTM.
- On each timestep *t* we have input $\boldsymbol{x}^{(t)}$ and hidden state $\boldsymbol{h}^{(t)}$ (no cell state).

Update gate: controls what parts of hi dden state are updated vs preserved

$$\boldsymbol{u}^{(t)} = \sigma\left(\boldsymbol{W}_u \boldsymbol{h}^{(t-1)} + \boldsymbol{U}_u \boldsymbol{x}^{(t)} + \boldsymbol{b}_u\right)$$

Reset gate: controls what parts of previous hidden state are used to compute new content

$$\boldsymbol{r}^{(t)} = \sigma\left(\boldsymbol{W}_r \boldsymbol{h}^{(t-1)} + \boldsymbol{U}_r \boldsymbol{x}^{(t)} + \boldsymbol{b}_r\right)$$

New hidden state content: reset gate selects useful parts of prev hidden st ate. Use this and current input to co mpute new hidden content.

$$\tilde{\boldsymbol{h}}^{(t)} = \tanh\left(\boldsymbol{W}_h(\boldsymbol{r}^{(t)} \circ \boldsymbol{h}^{(t-1)}) + \boldsymbol{U}_h \boldsymbol{x}^{(t)} + \boldsymbol{b}_h\right)$$

Hidden state: update gate simultaneou sly controls what is kept from previous hidden state, and what is updated to n ew hidden state content

$$\boldsymbol{h}^{(t)} = (1 - \boldsymbol{u}^{(t)}) \circ \boldsymbol{h}^{(t-1)} + \boldsymbol{u}^{(t)} \circ \tilde{\boldsymbol{h}}^{(t)}$$

How does this solve vanishing gradient? Lik e LSTM, GRU makes it easier to retain info lo ng-term (e.g. by setting update gate to 0)

LSTM vs GRU

- Researchers have proposed many gated RNN variants, but LSTM and GRU are the most widely-used
- The biggest difference is that GRU is quicker to compute and has fewer parameters
- There is no conclusive evidence that one consistently performs better than the other
- LSTM is a good default choice (especially if your data has particularly long dependencies, or you have lots of training data)
- Rule of thumb: start with LSTM, but switch to GRU if you want something more efficient

Is vanishing/exploding gradient just a RNN problem?

- No! It can be a problem for all neural architectures (including feed-forward and convolutional), especially very deep ones.
  - Due to chain rule / choice of nonlinearity function, gradient can become vanishingly small as it backpropagates
  - Thus, lower layers are learned very slowly (hard to train)
- Solution: lots of new deep feedforward/convolutional architectures that add more direct connections (thus allowing the gradient to flow)

For example:

- Residual connections aka "ResNet"
- Also known as skip-connections
- The identity connection preserves information by default
- This makes deep networks much easier to train

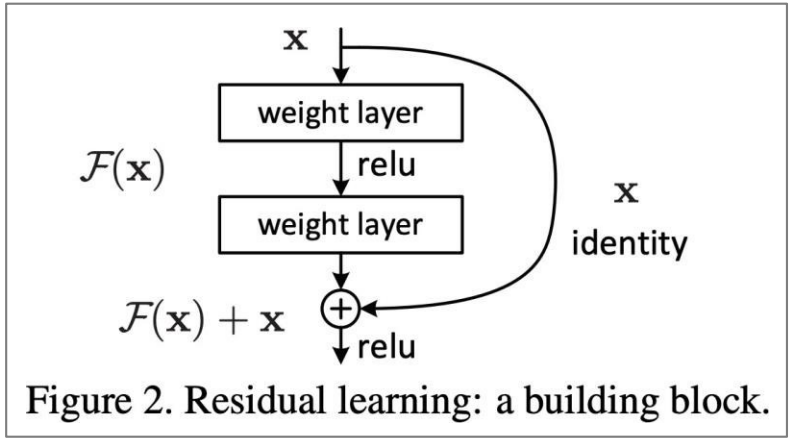


Figure 2. Residual learning: a building block.

Is vanishing/exploding gradient just a RNN problem?

- Solution: lots of new deep feedforward/convolutional architectures that add more direct connections (thus allowing the gradient to flow)

Other methods:

- Dense connections aka “DenseNet”
- Directly connect each layer to all future layers!

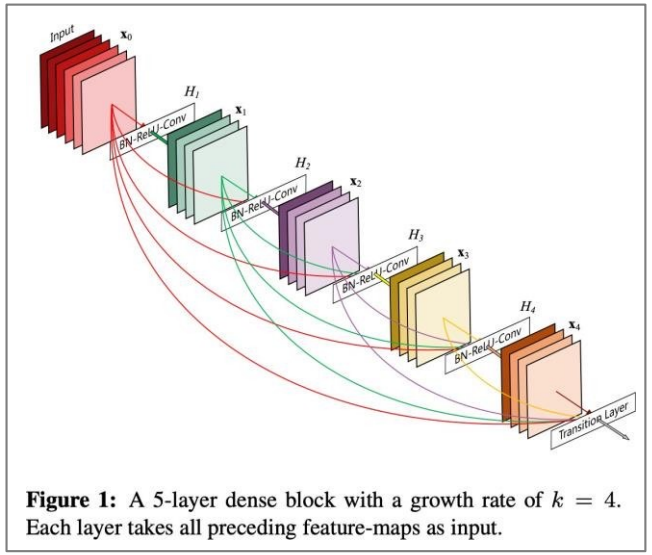
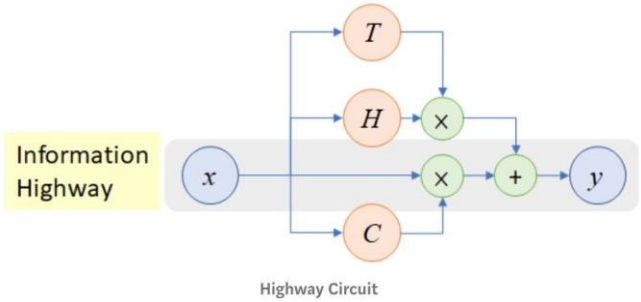


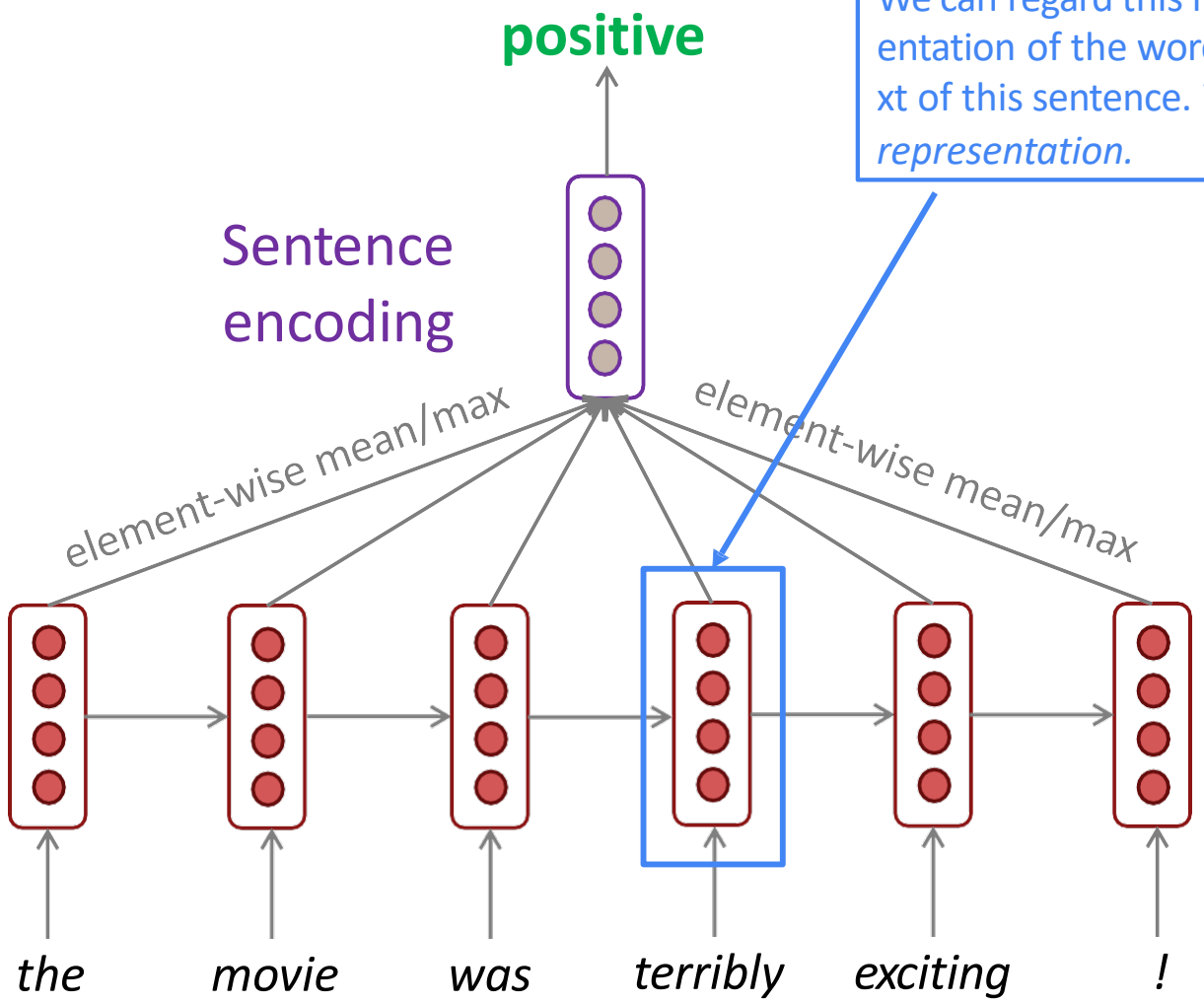
Figure 1: A 5-layer dense block with a growth rate of $k = 4$. Each layer takes all preceding feature-maps as input.

- Highway connections aka “HighwayNet”
- Similar to residual connections, but the identity connection vs the transformation layer is contr olled by a dynamic gate
- Inspired by LSTMs, but applied to deep feedforward/convolutional networks



Highway Circuit

Bidirectional and Multi-layer RNNs: motivation



We can regard this hidden state as a repres entation of the word *"terribly"* in the conte xt of this sentence. We call this a *contextual representation.*

These contextual repre sentations only contai n information about th e *left* context (e.g. *"th e movie was"*).

What about *right* context?

In this example, *"exci ting"* is in the right c ontext and this modifies the meaning of *"terribly"* (from negative to positive)

Bidirectional RNNs

- Note: bidirectional RNNs are only applicable if you have access to the entire input sequence
  - They are **not** applicable to Language Modeling, because in LM you *only* have left context available.

- If you do have entire input sequence (e.g., any kind of encoding), bidirectionality is powerful (you should use it by default).

- For example, BERT (**Bidirectional** Encoder Representations from Transformers) is a powerful pretrained contextual representation system built on bidirectionality.
  - You will learn more about transformers include BERT in a couple of weeks!

Multi-layer RNNs

- RNNs are already “deep” on one dimension (they unroll over many timesteps)
- We can also make them “deep” in another dimension by applying multiple RNNs – this is a multi-layer RNN.
- This allows the network to compute more complex representations
  - The lower RNNs should compute lower-level features and the higher RNNs should compute higher-level features.
- Multi-layer RNNs are also called *stacked RNNs*.

Multi-layer RNNs in practice

- High-performing RNNs are often multi-layer (but aren't as deep as convolutional or feed-forward networks)
- For example: In a 2017 paper, Britz et al find that for Neural Machine Translation, 2 to 4 layers is best for the encoder RNN, and 4 layers is best for the decoder RNN
  - Usually, skip-connections/dense-connections are needed to train deeper RNNs (e.g., 8 layers)
- Transformer-based networks (e.g., BERT) are usually deeper, like 12 or 24 layers.
  - You will learn about Transformers later; they have a lot of skipping-like connections

Machine Translation

Machine Translation (MT) is the task of translating a sentence *x* from one language (the source language) to a sentence *y* in another language (the target language).

x: *L'homme est né libre, et partout il est dans les fers*

y: *Man is born free, but everywhere he is in chains*

– Rousseau

1990s-2010s: Statistical Machine Translation

- Core idea: Learn a probabilistic model from data
- Suppose we're translating French → English.
- We want to find best English sentence *y*, given French sentence *x*

$$\text{argmax}_y P(y|x)$$

- Use Bayes Rule to break this down into two components to be learned separately:

$$= \text{argmax}_y \underbrace{P(x|y)}_{\text{Translation Model}} \underbrace{P(y)}_{\text{Language Model}}$$

Translation Model

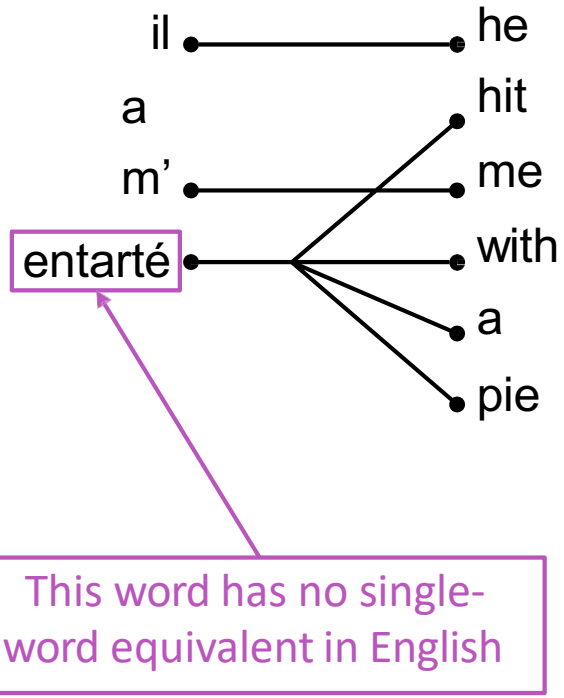
Models how words and phrases should be translated (*fidelity*). Learnt from parallel data.

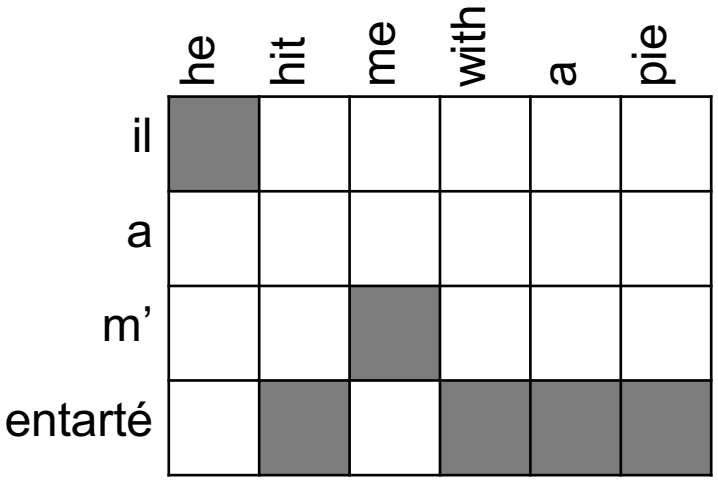
Language Model

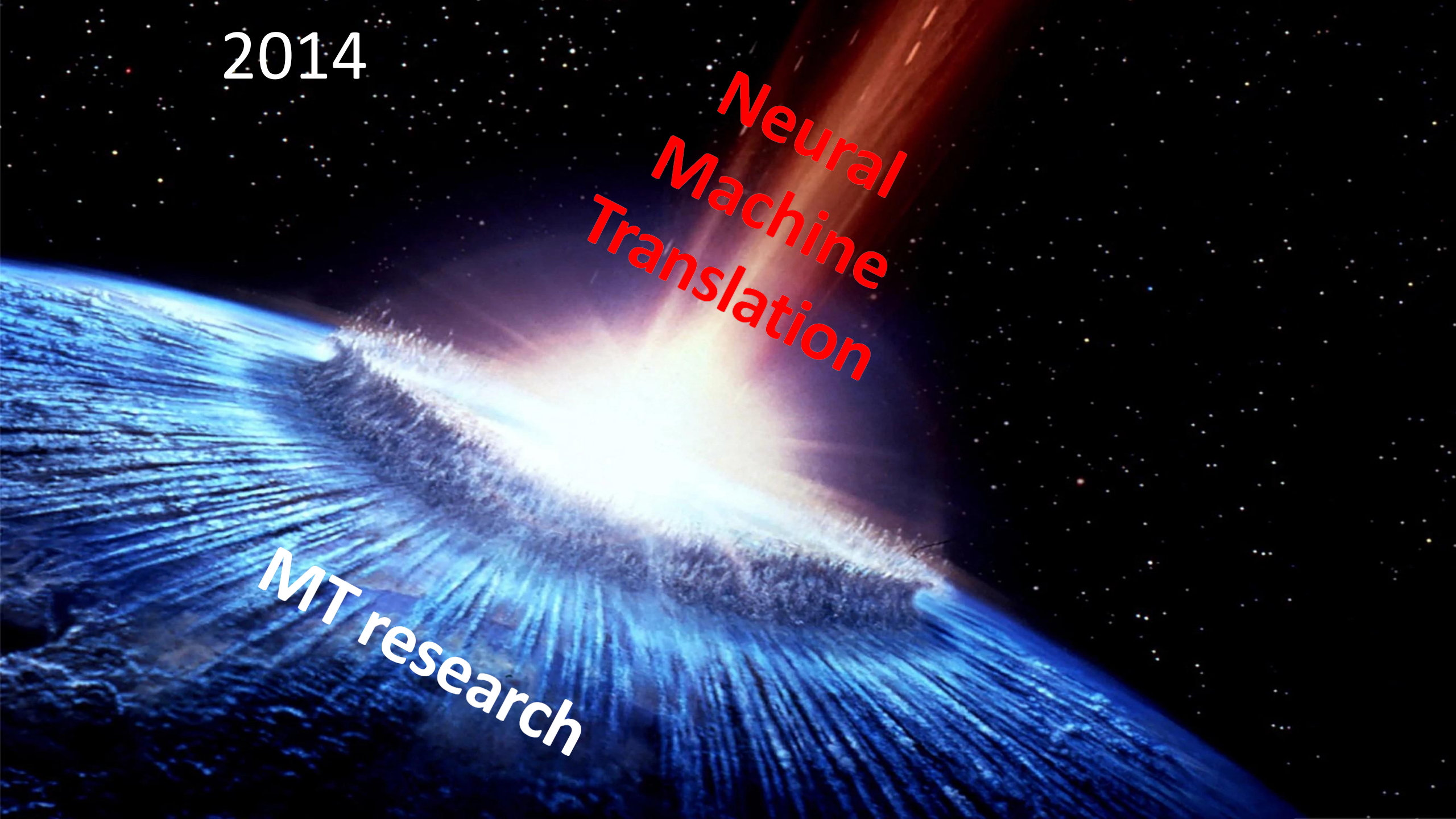
Models how to write good English (*fluency*). Learnt from monolingual data.

Alignment is complex

Some words are very fertile!

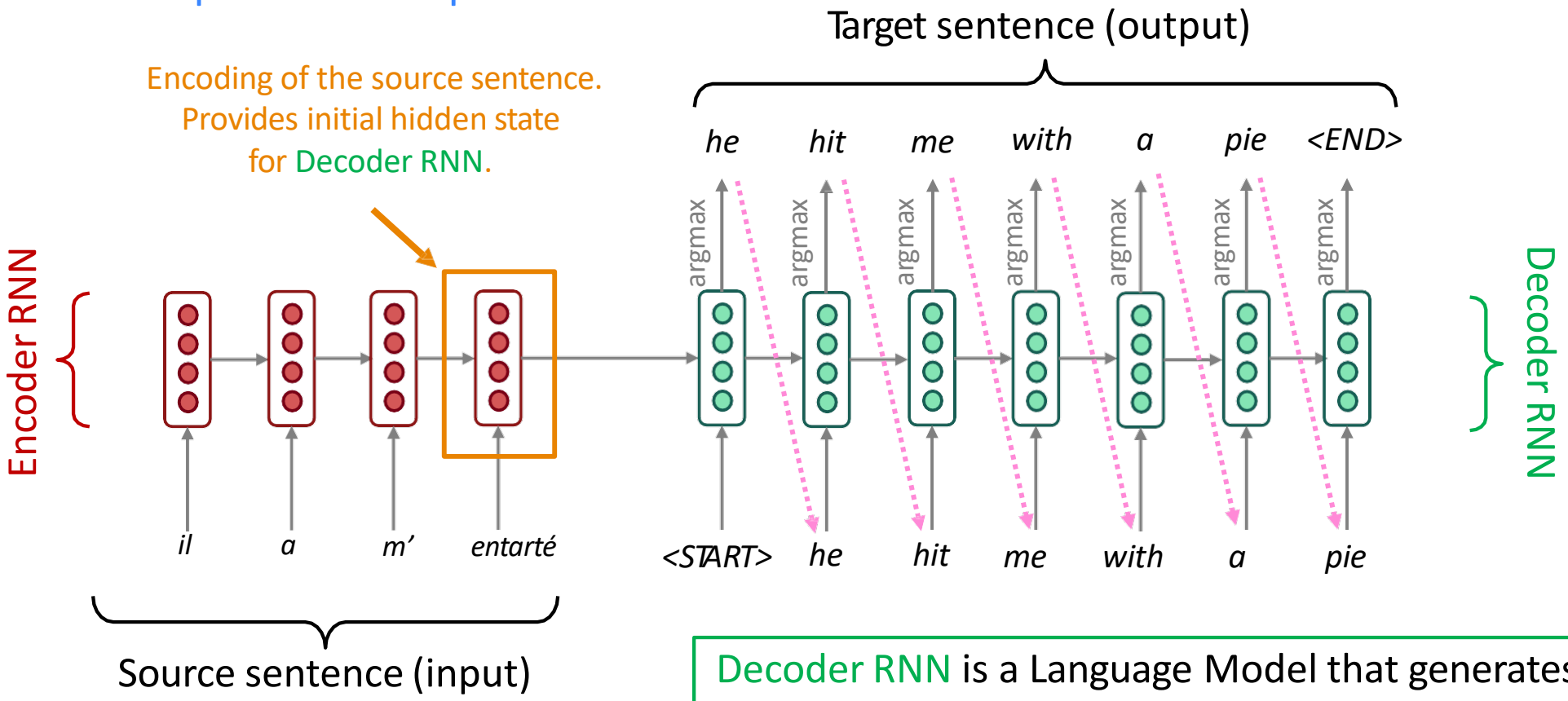





2014
Neural
Machine
Translation
MT research

Neural Machine Translation (NMT)

The sequence-to-sequence model

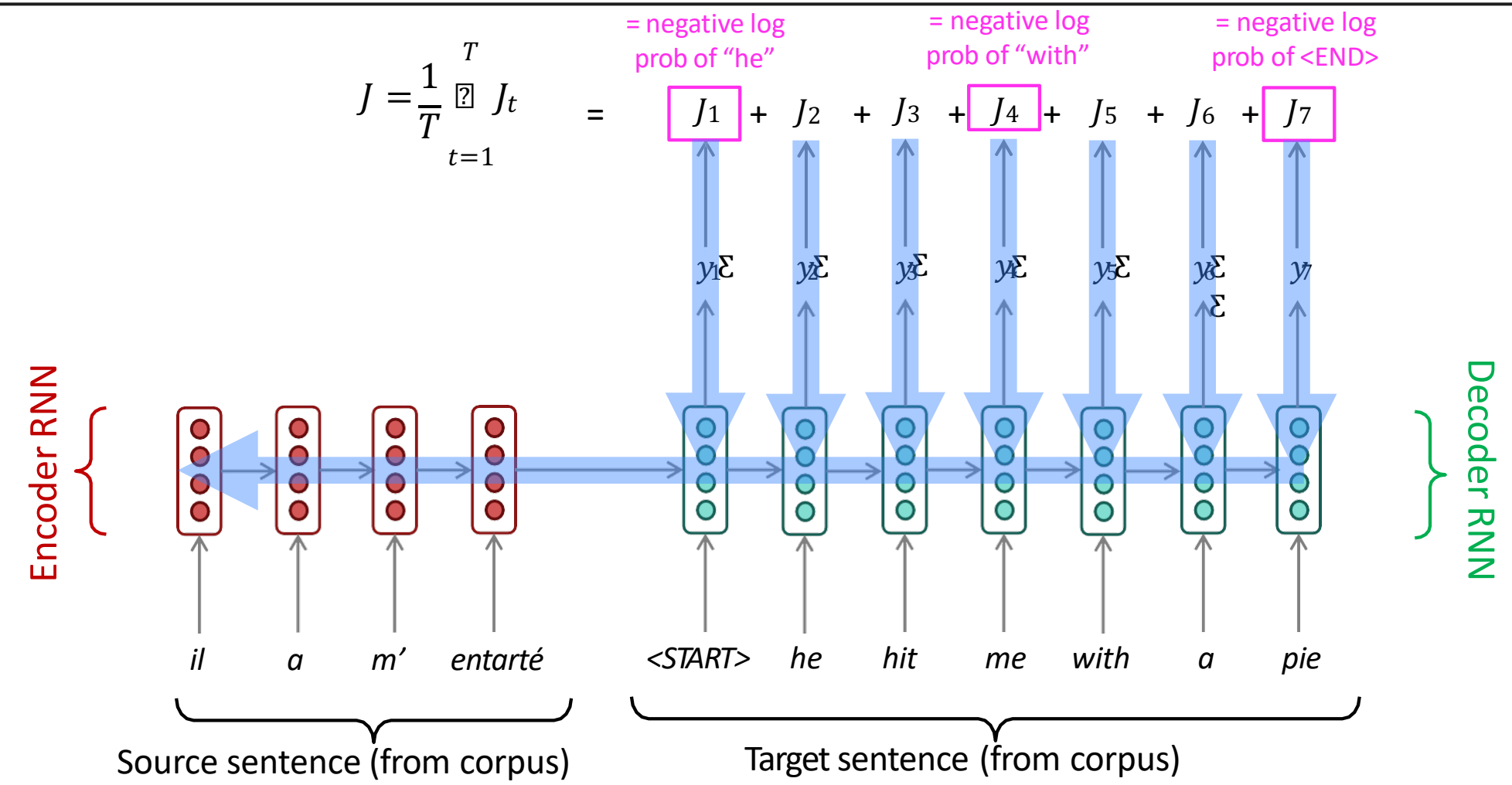


Encoder RNN produces an encoding of the source sentence.

Decoder RNN is a Language Model that generates target sentence, *conditioned on encoding*.

Note: This diagram shows **test time** behavior: decoder output is fed in ⋯→ as next step's input

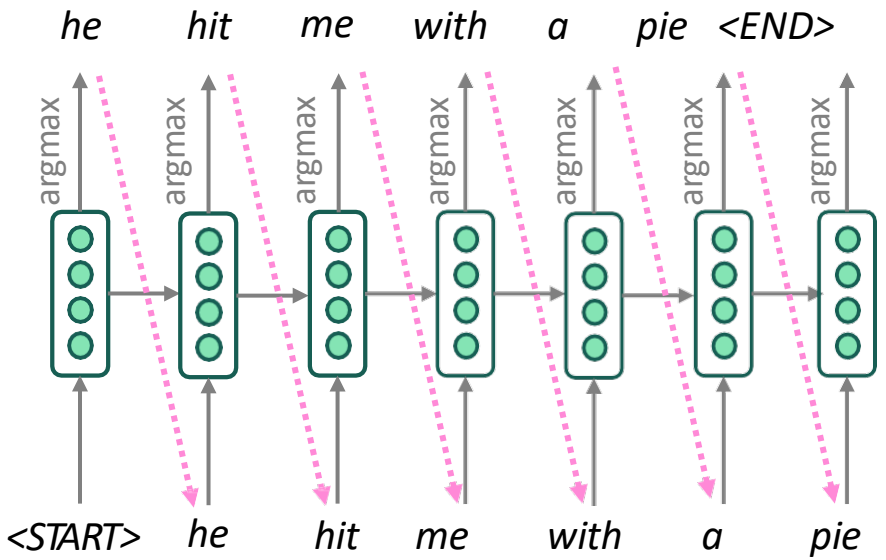
Training a Neural Machine Translation system



Seq2seq is optimized as a **single system.** Backpropagation operates "*end-to-end*".

Greedy decoding

- We saw how to generate (or “decode”) the target sentence by taking argmax on each step of the decoder



- This is greedy decoding (take most probable word on each step)
- **Problems with this method?**

Problems with greedy decoding

- Greedy decoding has no way to undo decisions!
  - Input: *il a m'entarté* *(he hit me with a pie)*
  - → *he* ____
  - → *he hit* ____
  - → *he hit a* ____ *(whoops! no going back now…)*
- How to fix this?

Exhaustive search decoding

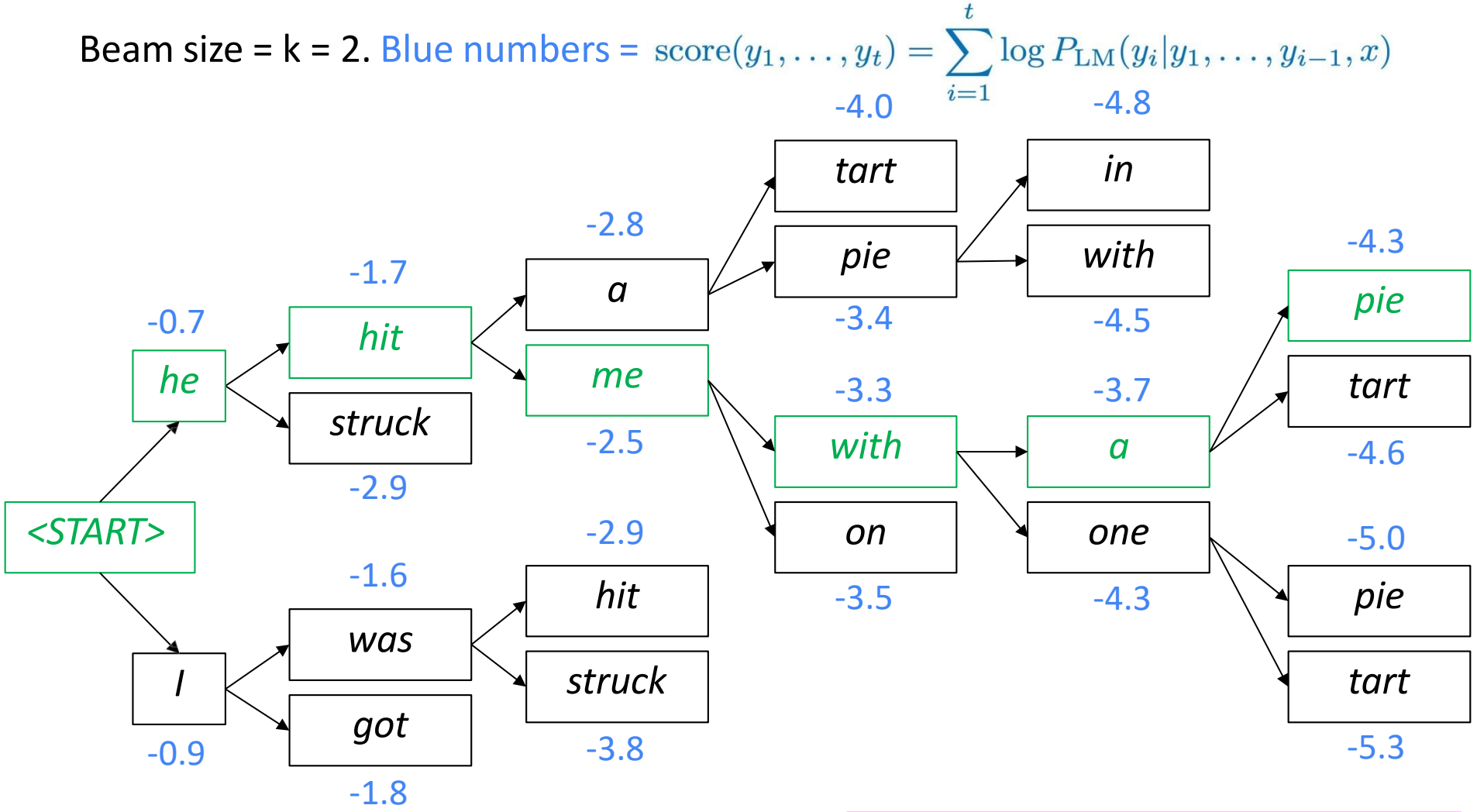
- Ideally, we want to find a (length *T*) translation *y* that maximizes

$$P(y|x) = P(y_1|x)\,P(y_2|y_1,x)\,P(y_3|y_1,y_2,x)\ldots,P(y_T|y_1,\ldots,y_{T-1},x)$$
$$= \prod_{t=1}^{T} P(y_t|y_1,\ldots,y_{t-1},x)$$

- We could try computing all possible sequences *y*
  - This means that on each step *t* of the decoder, we're tracking V^t possible partial translations, where *V* is vocab size
  - This $O(V^T)$ complexity is far too expensive!

Beam search decoding

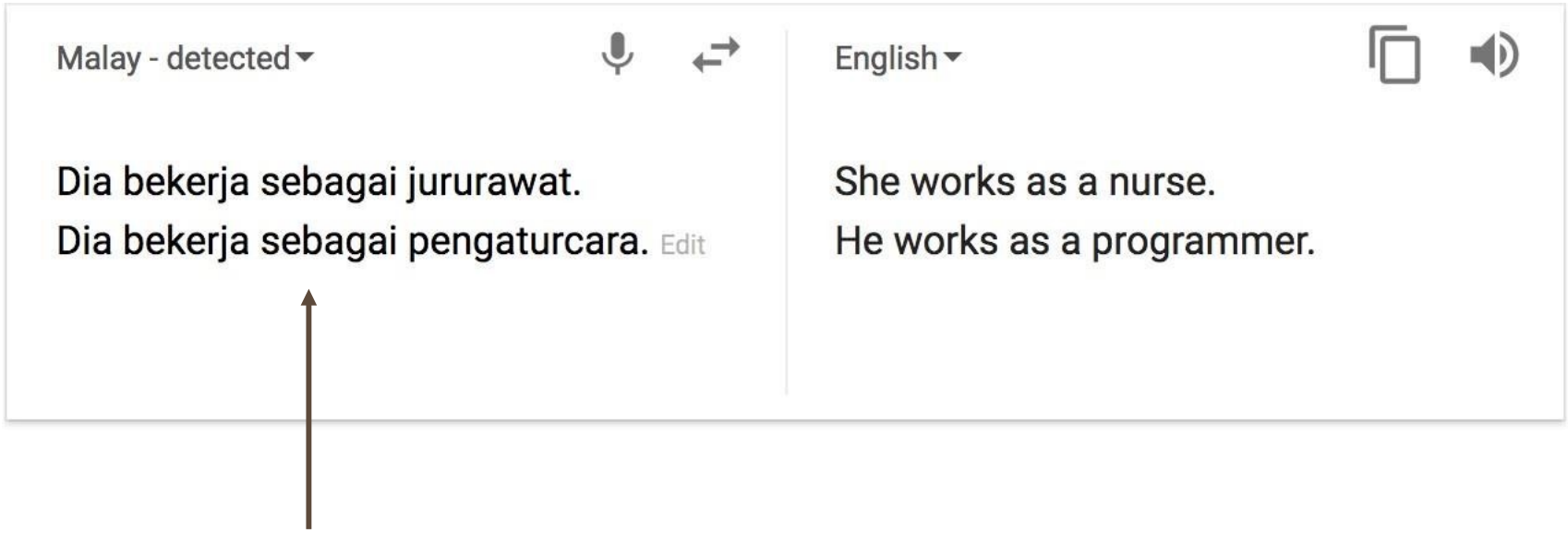
Beam size = k = 2. Blue numbers = $\text{score}(y_1, \ldots, y_t) = \sum_{i=1}^{t} \log P_{\text{LM}}(y_i | y_1, \ldots, y_{i-1}, x)$



Backtrack to obtain the full hypothesis

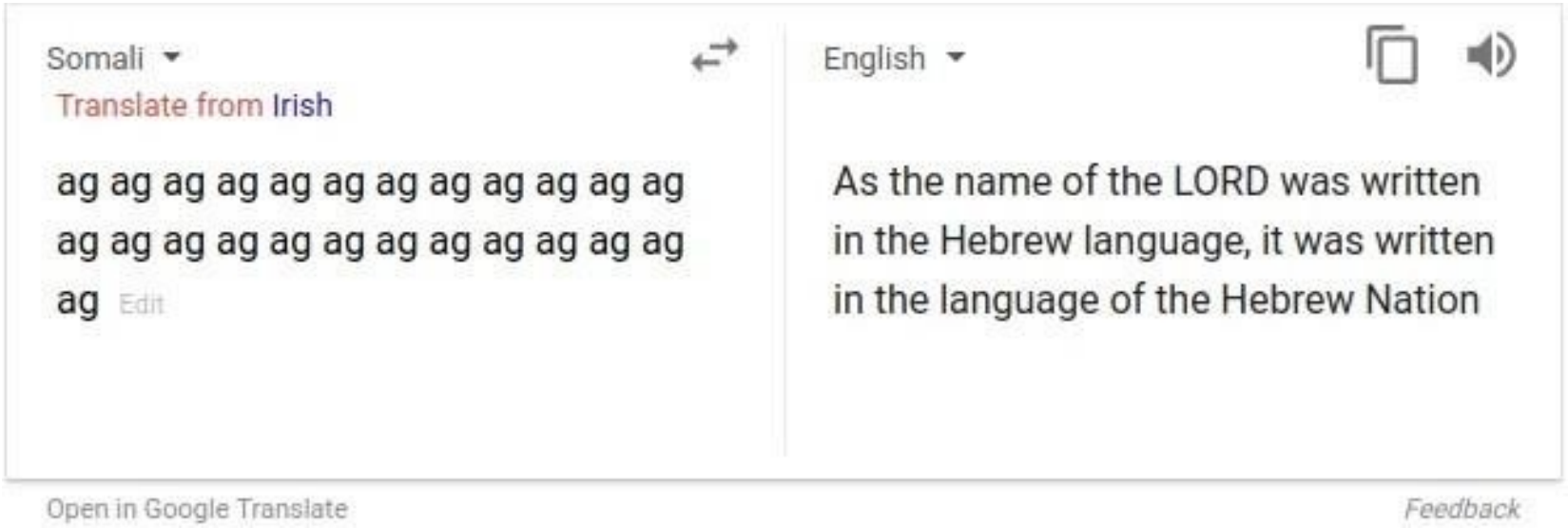
So, is Machine Translation solved?

- **Nope!**
- NMT picks up biases in training data



So, is Machine Translation solved?

- **Nope!**
- Uninterpretable systems do strange things
- (The example below is fixed in 2021)



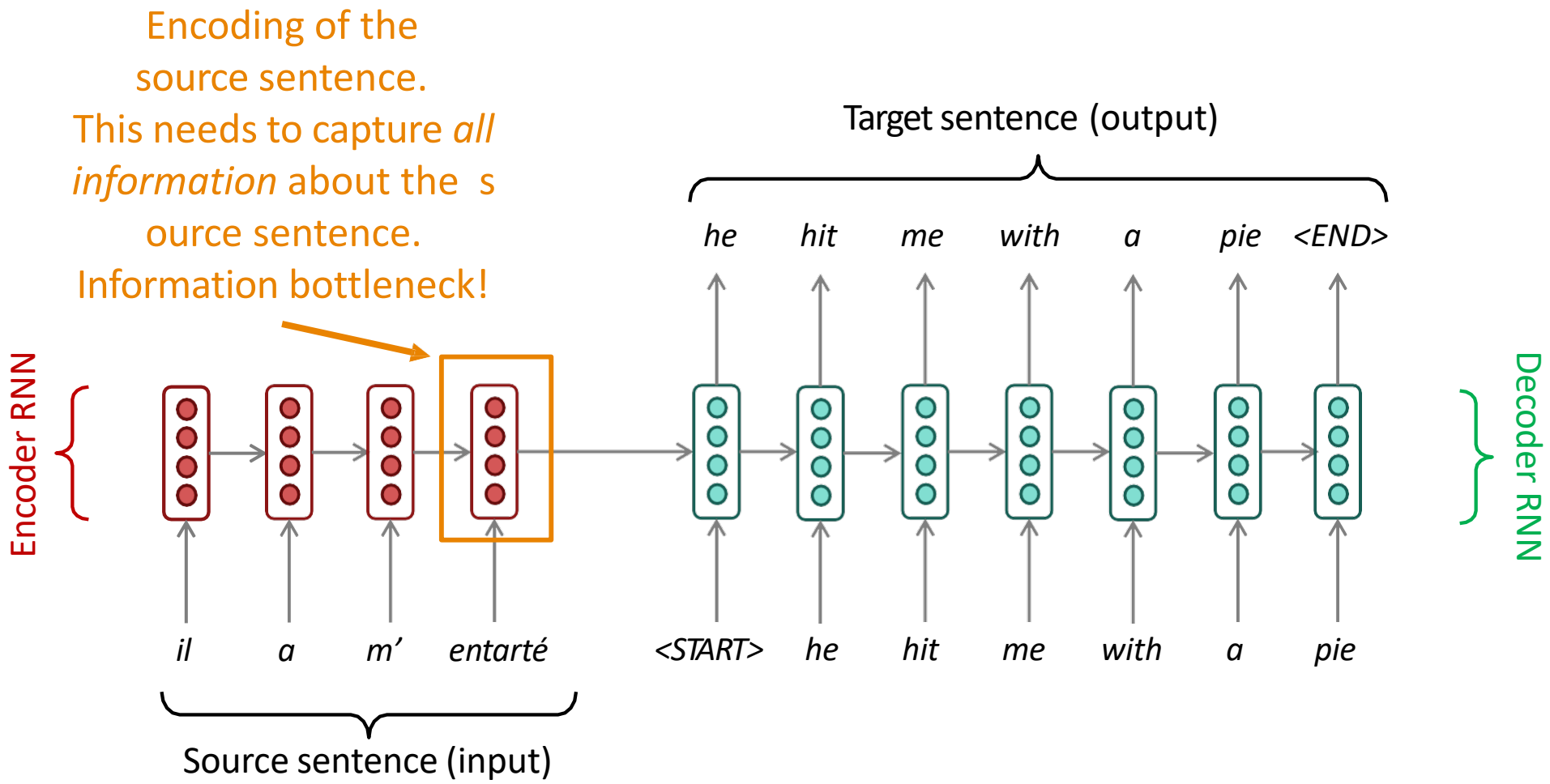
NMT research continues

NMT is a **flagship task** for NLP Deep Learning

- NMT research has pioneered many of the recent innovations of NLP Deep Learning
- In **2021**: NMT research continues to thrive
  - Researchers have found *many, many* improvements to the "vanilla" seq2seq NMT system we've just presented
  - But we'll present in a minute one improvement so integral that it is the new vanilla…

ATTENTION

Sequence-to-sequence: the bottleneck problem

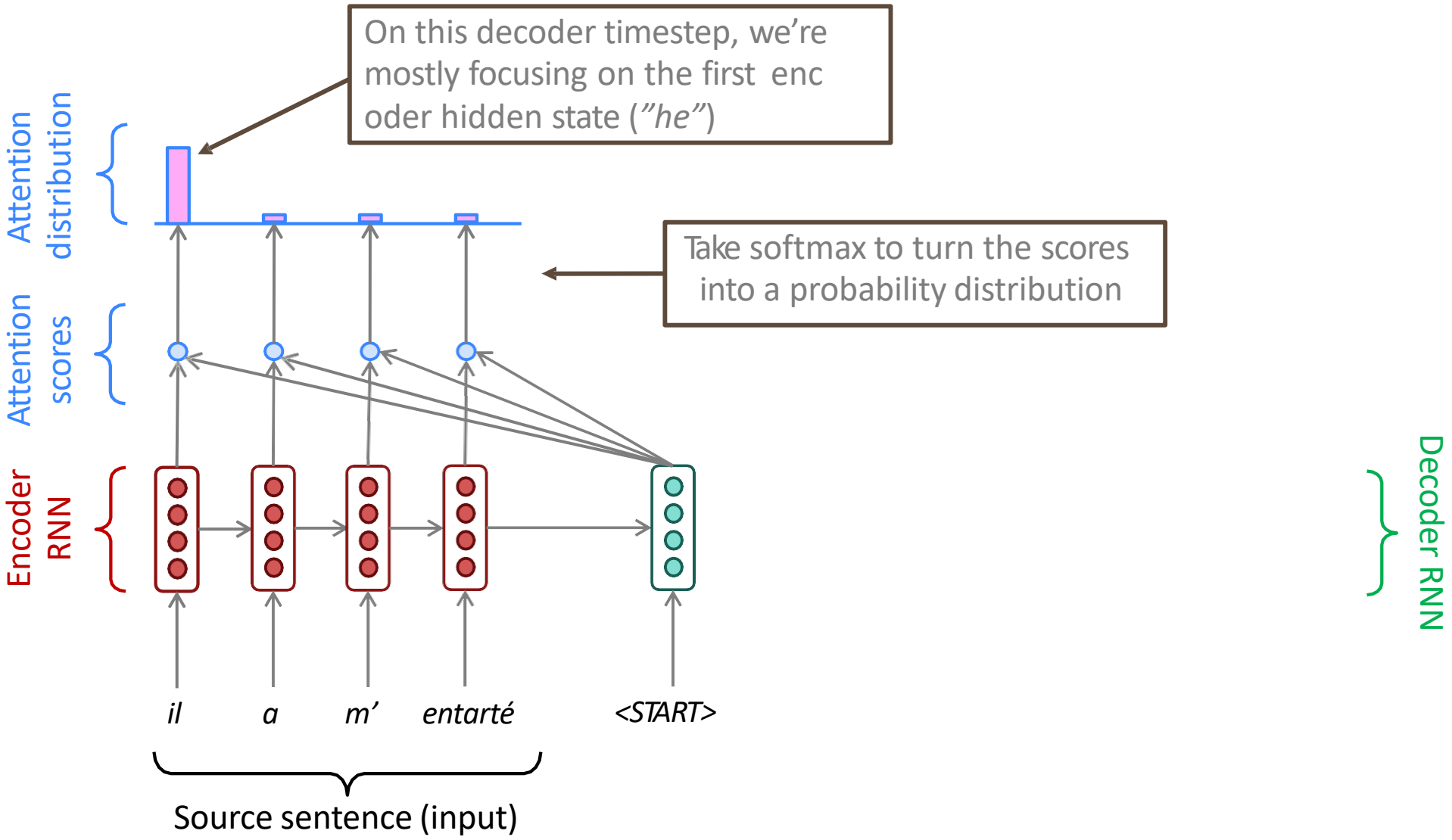


Attention

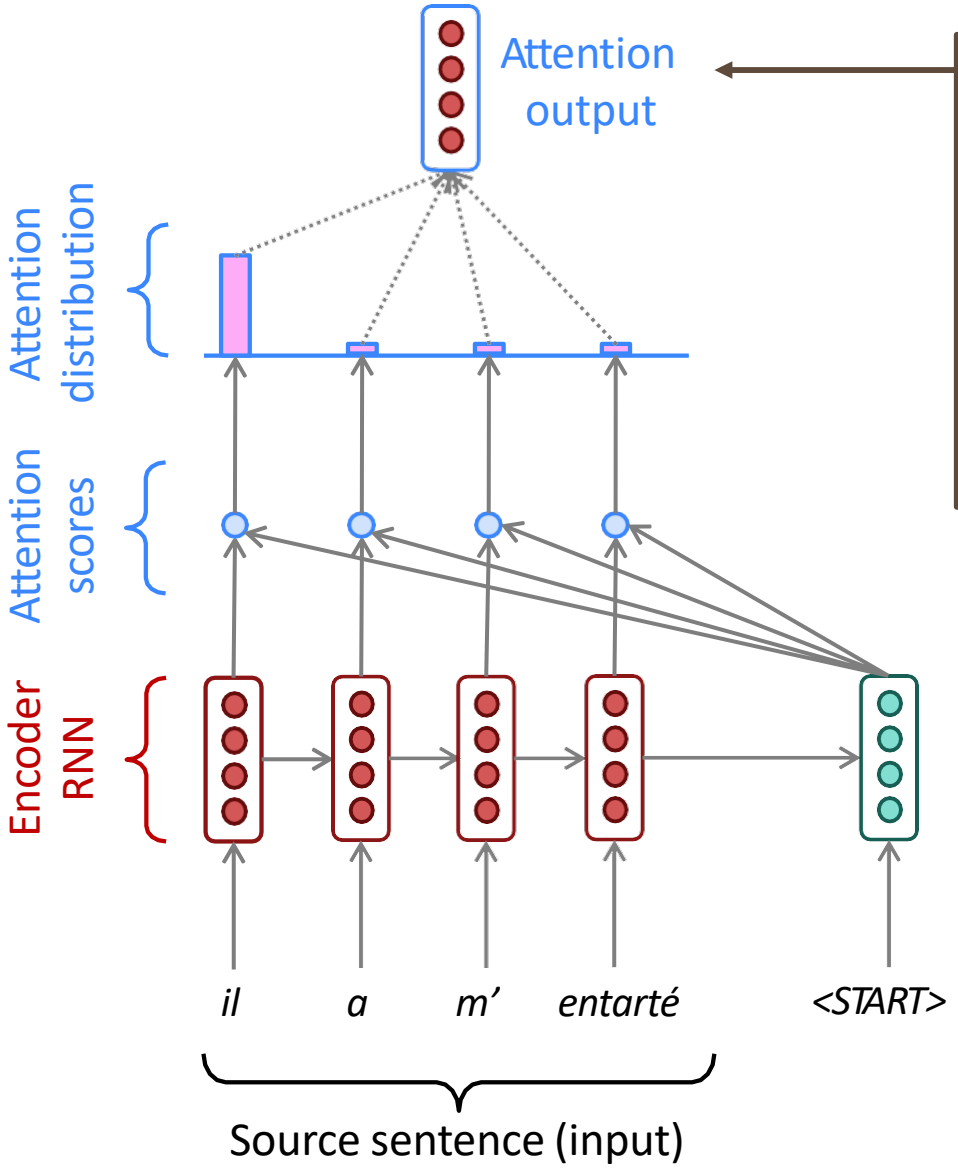
- **Attention** provides a solution to the bottleneck problem.
- Core idea: on each step of the decoder, use *direct connection to the encoder* to *focus on a particular part* of the source sequence

- First, we will show via diagram (no equations), then we will show with equations

Sequence-to-sequence with attention



Sequence-to-sequence with attention

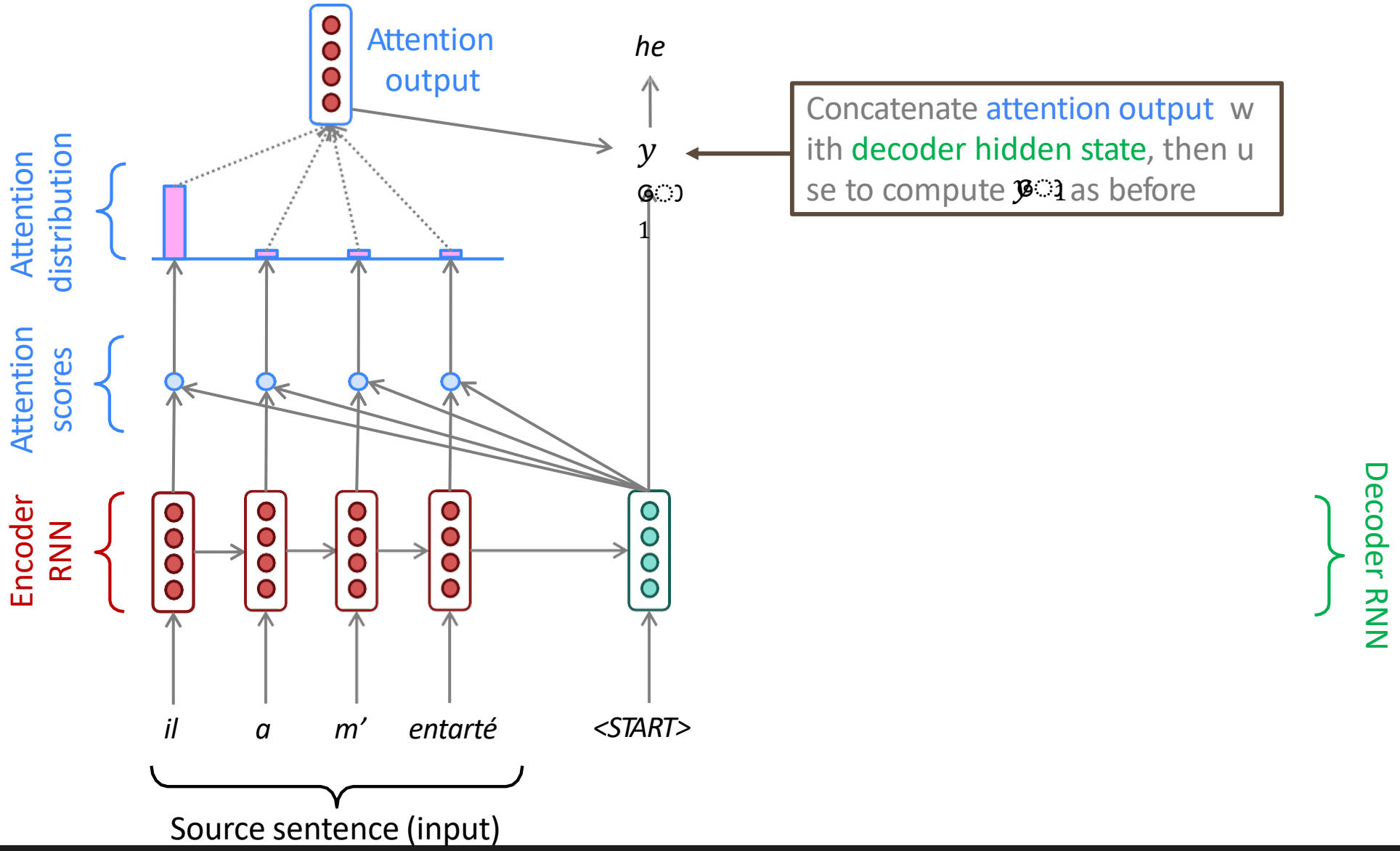


Use the attention distribution to take a **weighted sum** of the encoder hidden states.

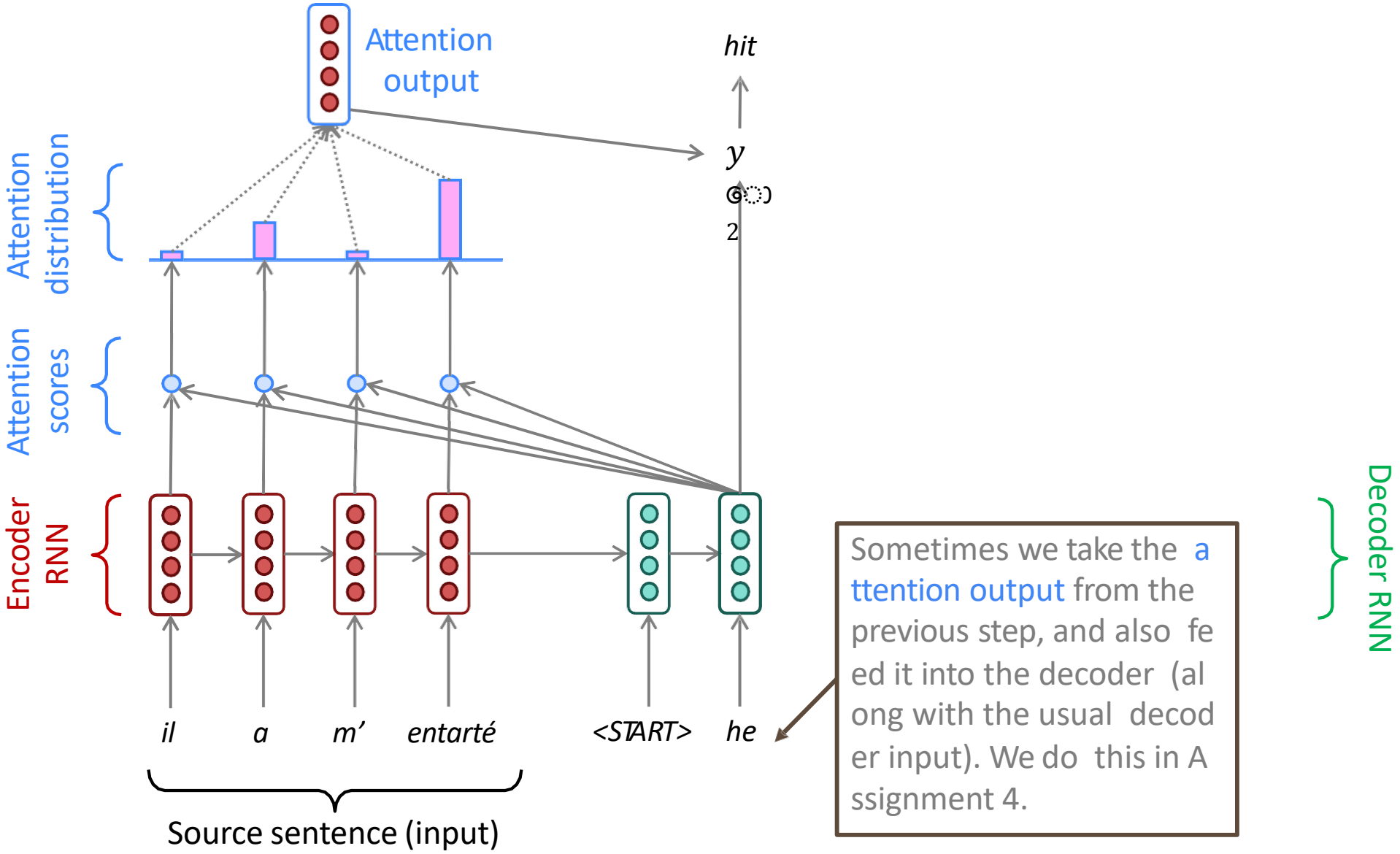
The attention output mostly contains in f ormation from the hidden states that re ceived high attention.

Decoder RNN

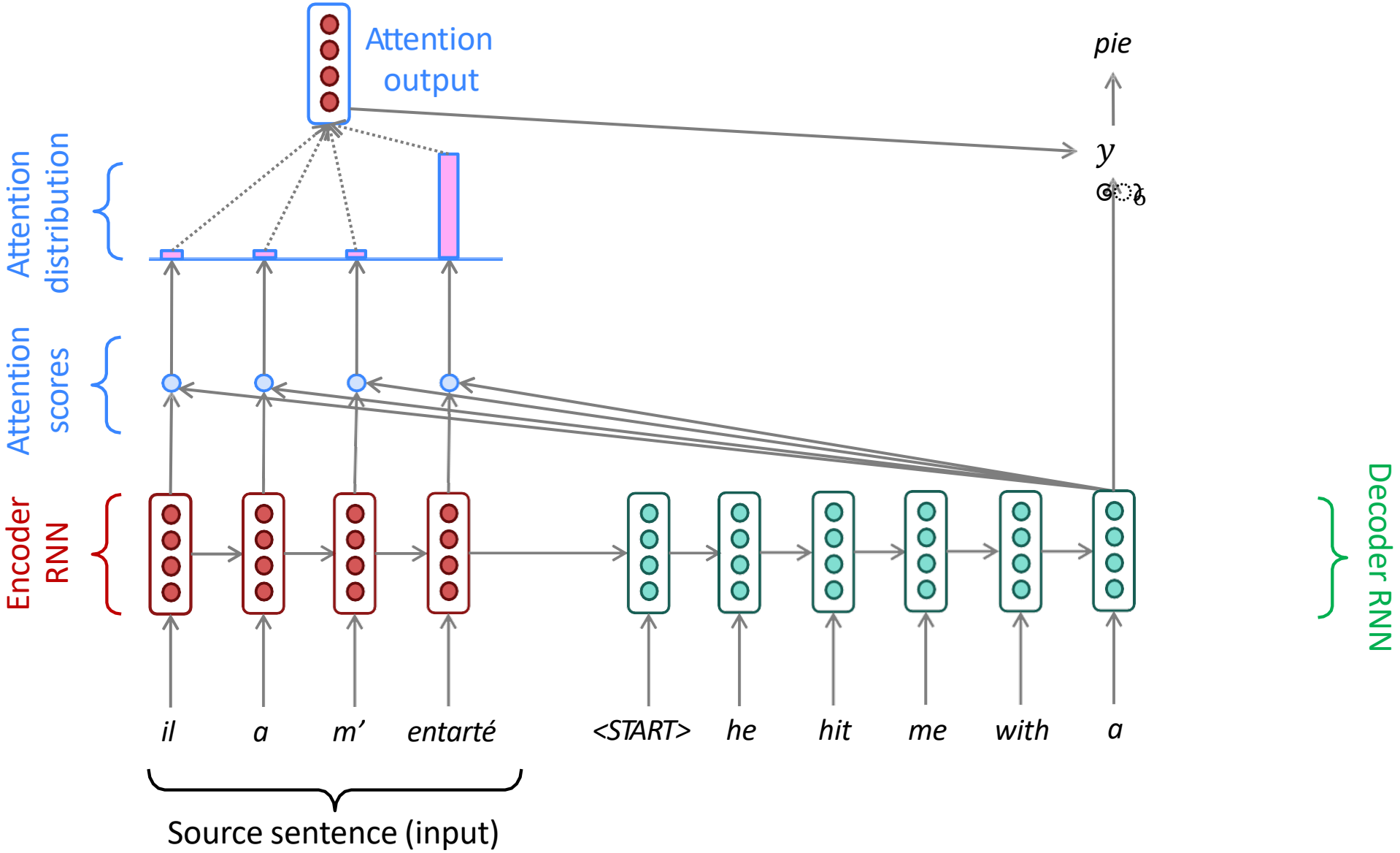
Sequence-to-sequence with attention



Sequence-to-sequence with attention



Sequence-to-sequence with attention



Attention: in equations

- We have encoder hidden states $h_1, \ldots, h_N \in \mathbb{R}^h$
- On timestep *t*, we have decoder hidden state $s_t \in \mathbb{R}^h$
- We get the attention scores e^t for this step:

$$\boldsymbol{e}^t = [\boldsymbol{s}_t^T \boldsymbol{h}_1, \ldots, \boldsymbol{s}_t^T \boldsymbol{h}_N] \in \mathbb{R}^N$$

- We take softmax to get the attention distribution α^t for this step (this is a probability distribution and sums to 1)

$$\alpha^t = \text{softmax}(\boldsymbol{e}^t) \in \mathbb{R}^N$$

- We use α^t to take a weighted sum of the encoder hidden states to get the attention output $\boldsymbol{a}_t$

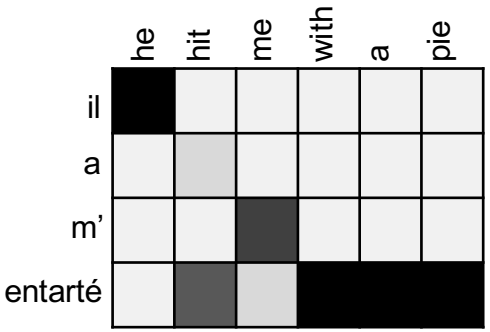
$$\boldsymbol{a}_t = \sum_{i=1}^{N} \alpha_i^t \boldsymbol{h}_i \in \mathbb{R}^h$$

- Finally we concatenate the attention output $\boldsymbol{a}_t$ with the decoder hidden state s_t and proceed as in the non-attention seq2seq model

$$[\boldsymbol{a}_t; \boldsymbol{s}_t] \in \mathbb{R}^{2h}$$

Attention is great

- **Attention significantly improves NMT performance**
  - It's very useful to allow decoder to focus on certain parts of the source
- **Attention solves the bottleneck problem**
  - Attention allows decoder to look directly at source; bypass bottleneck
- **Attention helps with vanishing gradient problem**
  - Provides shortcut to faraway states
- **Attention provides some interpretability**
  - By inspecting attention distribution, we can see what the decoder was focusing on
  - We get (soft) alignment for free!
  - This is cool because we never explicitly trained an alignment system
  - The network just learned alignment by itself



Attention is a general Deep Learning technique

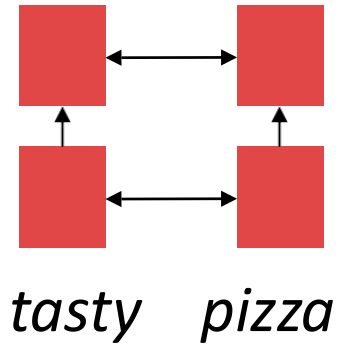
- We've seen that attention is a great way to improve the sequence-to-sequence model for Machine Translation.
- However: You can use attention in many architectures (not just seq2seq) and many tasks (not just MT)

- **More general definition of attention**:
  - Given a set of vector *values*, and a vector *query*, **attention** is a technique to compute a weighted sum of the values, dependent on the query.

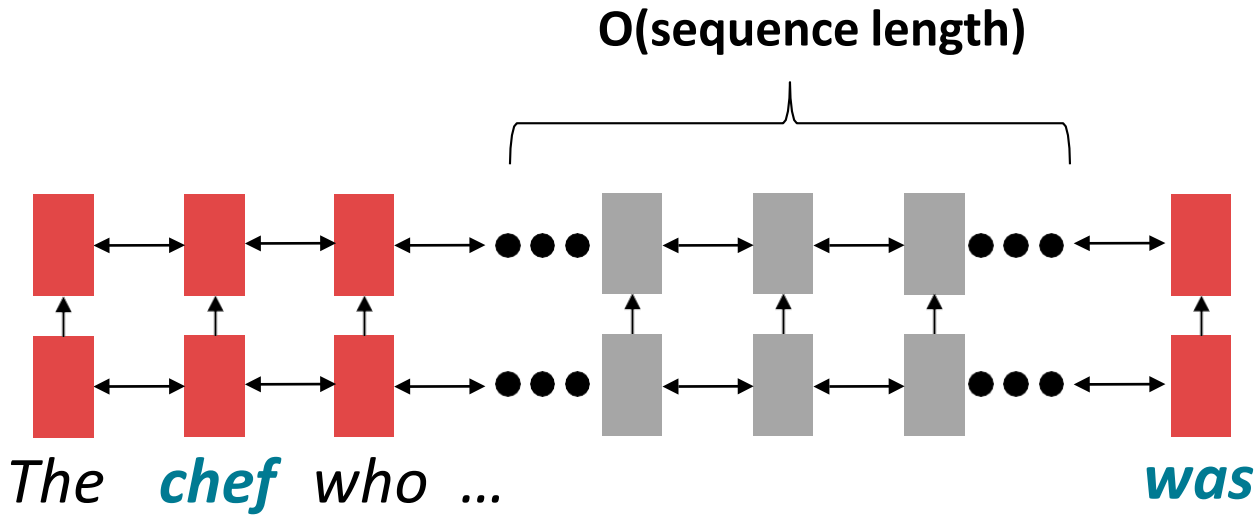
- We sometimes say that the query *attends to* the values.
- For example, in the seq2seq + attention model, each decoder hidden state (query) *attends to* all the encoder hidden states (values).

Issues with recurrent models: Linear interaction distance

- RNNs are unrolled “left-to-right”.
- This encodes linear locality: a useful heuristic!
  - Nearby words often affect each other’s meanings

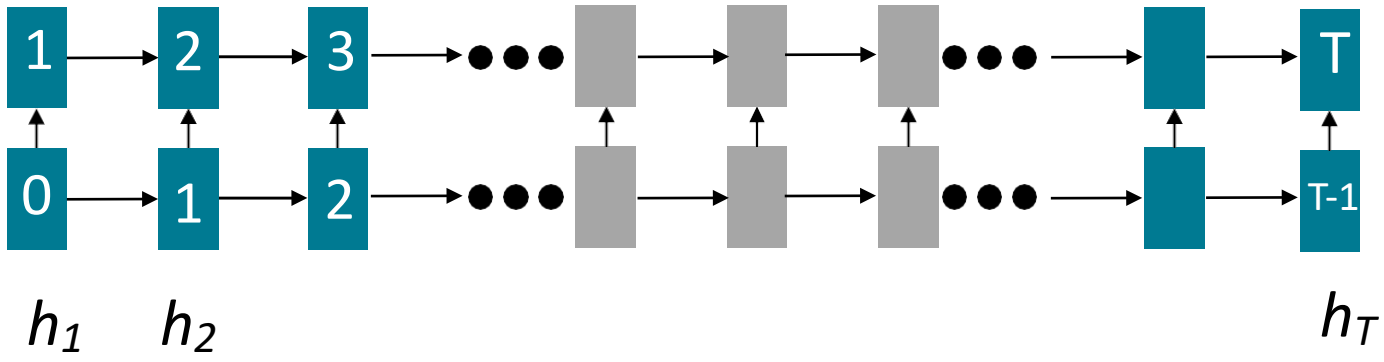


- **Problem:** RNNs take **O(sequence length)** steps for distant word pairs to interact.



Issues with recurrent models: Lack of parallelizability

- Forward and backward passes have **O(sequence length)** unparallelizable operations
  - GPUs can perform a bunch of independent computations at once!
  - But future RNN hidden states can't be computed in full before past RNN hidden states have been computed
  - Inhibits training on very large datasets!



Numbers indicate min # of steps before a state can be computed

Self-Attention

- Recall: Attention operates on **queries**, **keys**, and **values.**
  - We have some **queries** $q_1, q_2, \ldots, q_T$. Each query is $q \in \mathbb{R}^d$
  - We have some **keys** $k_1, k_2, \ldots, k_T$. Each key is $k_i \in \mathbb{R}^d$
  - We have some **values** $v_1, v_2, \ldots, v_T$. Each value is $v_i \in \mathbb{R}^d$

The number of queries can differ from the number of keys and values in practice.

- In **self-attention**, the queries, keys, and values are drawn from the same source.
  - For example, if the output of the previous layer is $x_1, \ldots, x_T$, (one vec per word) we could let $v_i = k_i = q_i = x_i$ (that is, use the same vectors for all of them!)
- The (dot product) self-attention operation is as follows:

$$e_{ij} = q_i^\top k_j$$

Compute **key-query** affinities

$$\alpha_{ij} = \frac{\exp(e_{ij})}{\sum_{j'} \exp(e_{ij'})}$$

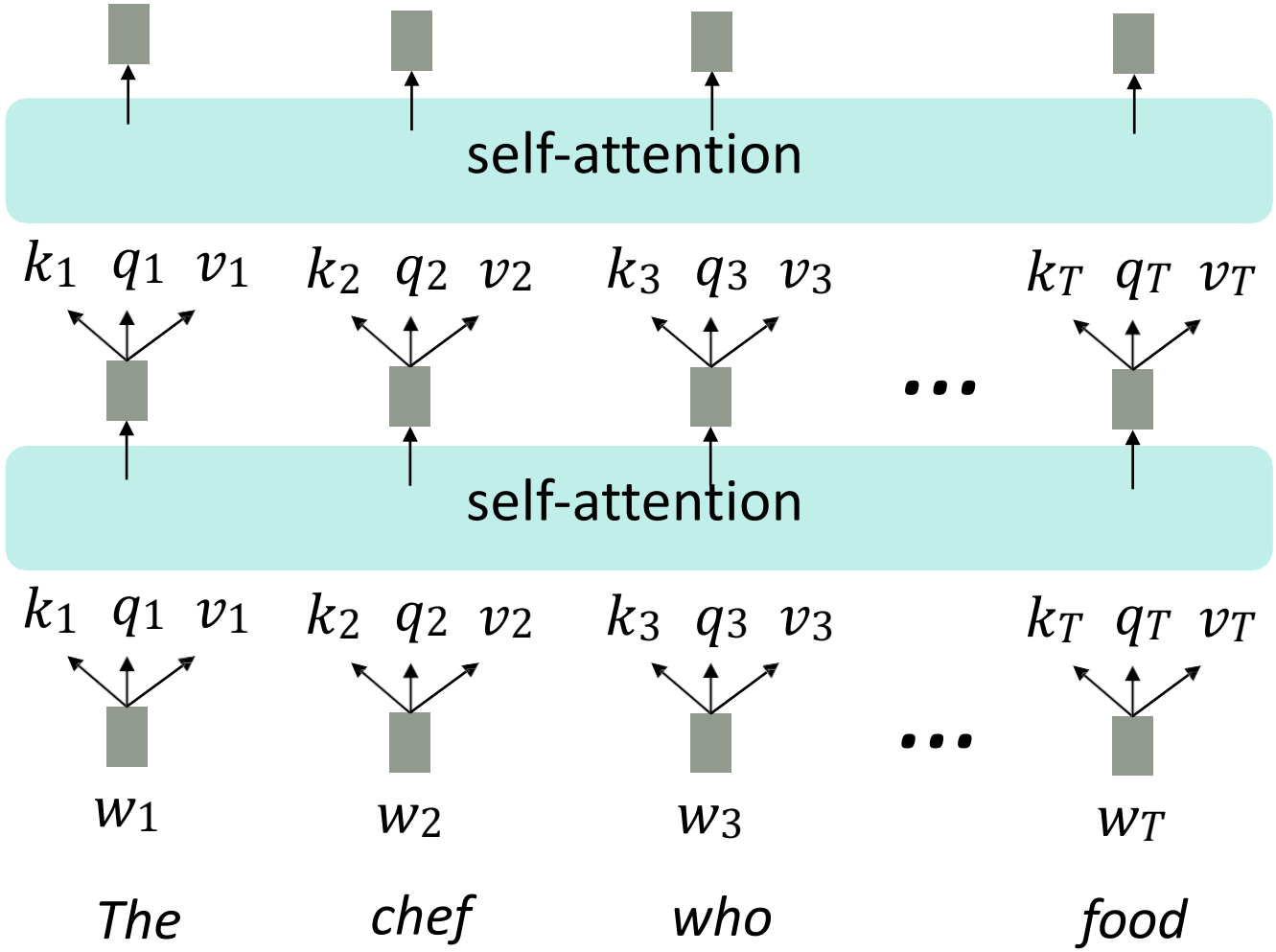
Compute attention weights from affinities (Softmax)

$$\text{output}_i = \sum_j \alpha_{ij} v_j$$

Compute outputs as weighted sum of **values**

Self-attention as an NLP building block

- In the diagram at the right, we have stacked self-attention blocks, like we might stack LSTM layers.
- Can self-attention be a drop-in replacement for recurrence?
- No. It has a few issues, which we'll go through.
- First, self-attention is an operation on **sets**. It has no inherent notion of order.



Self-attention doesn't know the order of its inputs.

Barriers and solutions for Self-Attention as a building block

Barriers

- Doesn't have an inherent notion of order!
- No nonlinearities for deep learning magic! It's all just weighted averages
- Need to ensure we don't "look at the future" when predicting a sequence
  - Like in machine translation
  - Or language modeling

Fixing the first self-attention problem: sequence order

- Since self-attention doesn't build in order information, we need to encode the order of the sentence in our keys, queries, and values.
- Consider representing each **sequence index** as a **vector**

$$p_i \in \mathbb{R}^d, \text{ for } i \in \{1,2,\dots,T\} \text{ are position vectors}$$

- Don't worry about what the p_i are made of yet!
- Easy to incorporate this info into our self-attention block: just add the p_i to our inputs!
- Let v, k, q be our old values, keys, and queries.

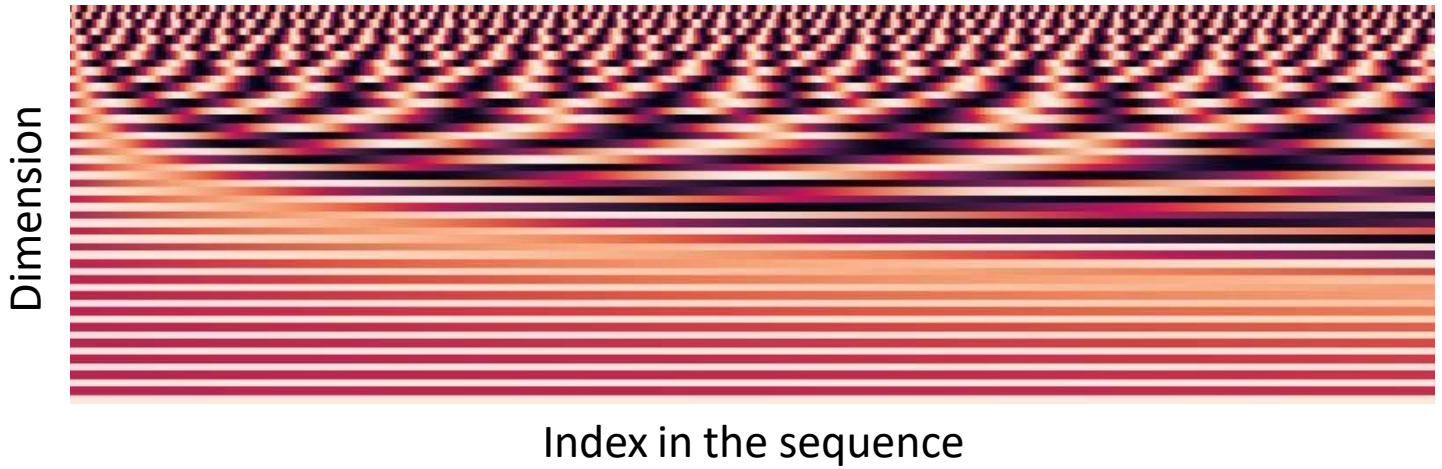
$$v_i = v + p_i$$
$$q_i = q + p_i$$
$$k_i = k + p_i$$

In deep self-attention networks, we do this at the first layer! You could concat enate them as well, but peo ple mostly just add…

Position representation vectors through sinusoids

- **Sinusoidal position representations:** concatenate sinusoidal functions of varying periods:

$$p_i = \begin{pmatrix} \sin(i/10000^{2*1/d}) \\ \cos(i/10000^{2*1/d}) \\ \vdots \\ \sin(i/10000^{2*\frac{d}{2}/d}) \\ \cos(i/10000^{2*\frac{d}{2}/d}) \end{pmatrix}$$



- Pros:
  - Periodicity indicates that maybe "absolute position" isn't as important
  - Maybe can extrapolate to longer sequences as periods restart!
- Cons:
  - Not learnable; also the extrapolation doesn't really work!

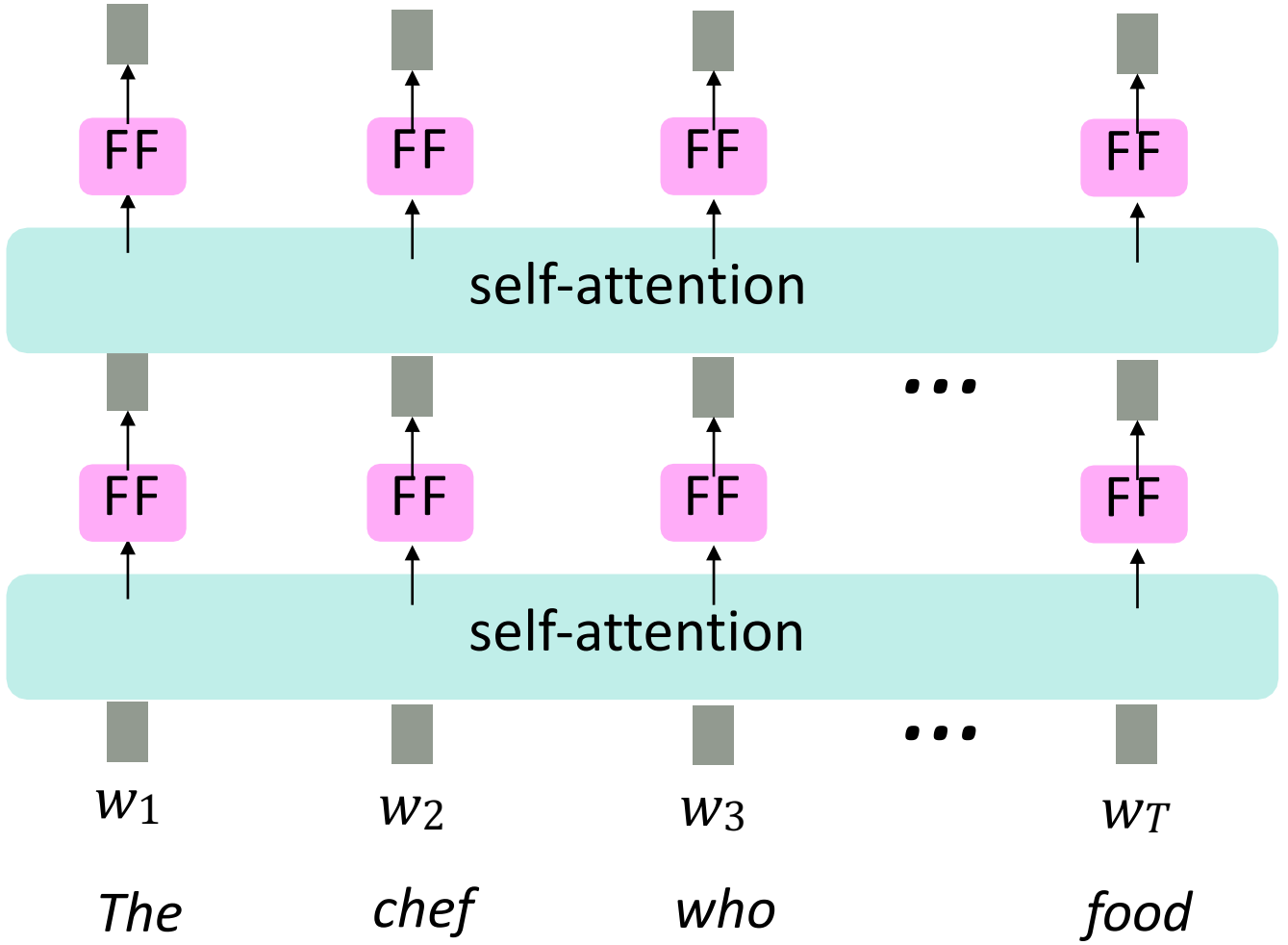
Image: https://timodenk.com/blog/linear-relationships-in-the-transformers-positional-encoding/

Adding nonlinearities in self-attention

- Note that there are no elementwise nonlinearities in self-attention; stac king more self-attention layers just r e-averages **value** vectors

- Easy fix: add a **feed-forward network** to post-process each output vector.

$$m_i = MLP(\text{output}_i)$$
$$= W_2 * \text{ReLU}\,(W_1 \times \text{output}_i + b_1) + b_2$$



Intuition: the FF network processes the result of attention

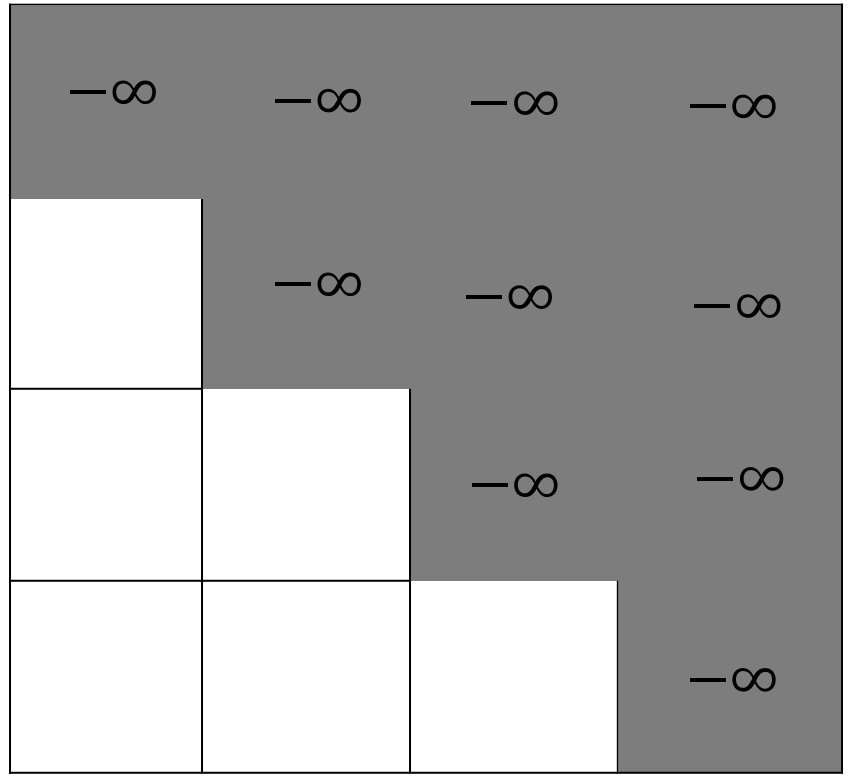
Masking the future in self-attention

- To use self-attention in **deco ders**, we need to ensure we c an't peek at the future.
- At every timestep, we could change the set of **keys and queries** to include only past words. (Inefficient!)
- To enable parallelization, we **mask out attention** to future words by setting attention s cores to $-\infty$.

$$e_{ij} = \begin{cases} q_i^\top k_j, j < i \\ -\infty, j \geq i \end{cases}$$

We can look at these (not greyed out) words

For encoding these words



[The matrix of e_{ij} values]

Attention weights automatically becomes 0

$$\alpha_{ij} = \frac{\exp(e_{ij})}{\sum_{j'} \exp(e_{ij'})}$$

Barriers and solutions for Self-Attention as a building block

Barriers	Solutions
• Doesn't have an inherent notion of order!	• Add position representations to the inputs
• No nonlinearities for deep learning magic! It's all just weighted averages	• Easy fix: apply the same feed forward network to each self-attention output.

• Need to ensure we don't "look at the future" when predicting a sequence
  • Like in machine translation
  • Or language modeling
	• Mask out the future by artificially setting attention weights to 0!

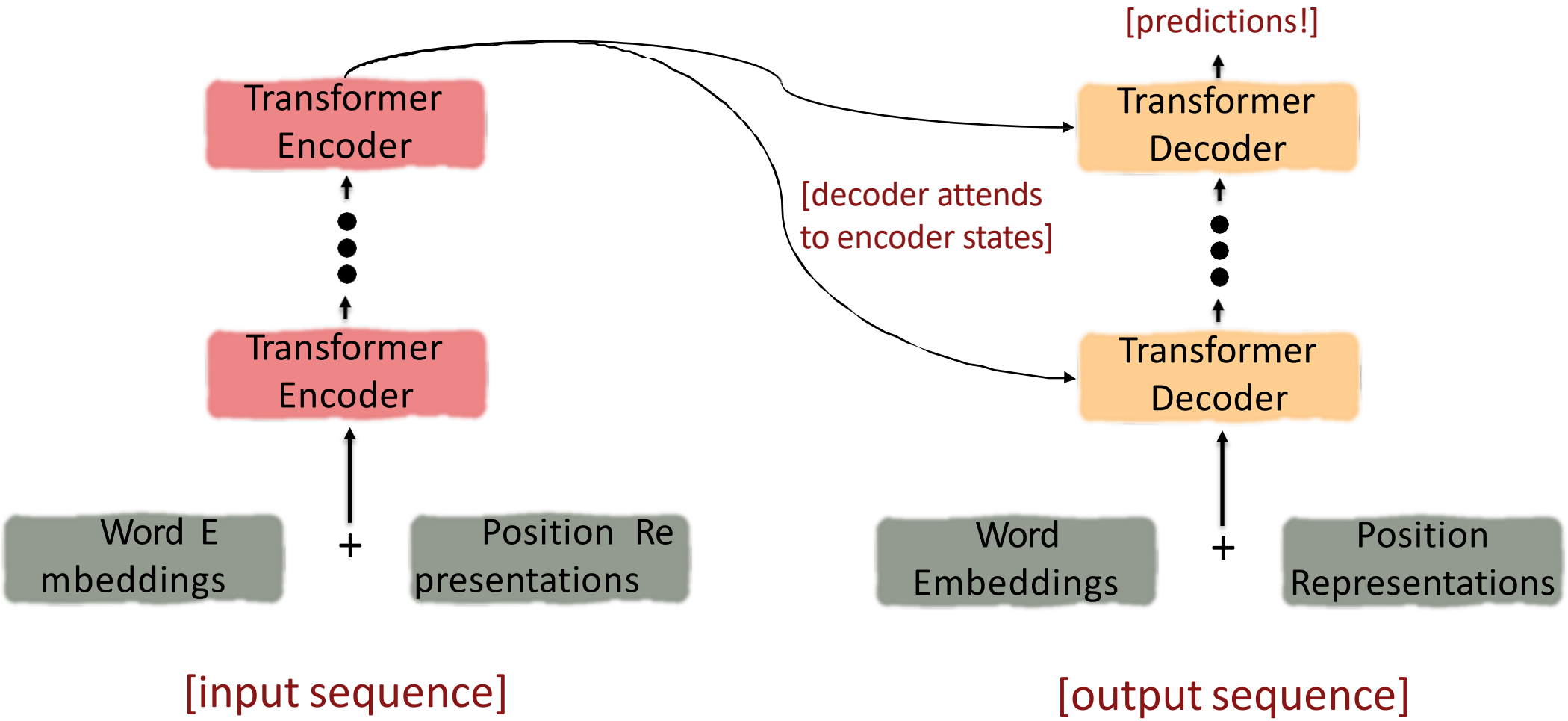
Necessities for a self-attention building block:

- **Self-attention**:
  - the basis of the method.
- **Position representations**:
  - Specify the sequence order, since self-attention is an unordered function of its inputs.
- **Nonlinearities**:
  - At the output of the self-attention block
  - Frequently implemented as a simple feed-forward network.
- **Masking**:
  - In order to parallelize operations while not looking at the future.
  - Keeps information about the future from “leaking” to the past.

- That’s it! But this is not the **Transformer** model we’ve been hearing about.

The Transformer Encoder-Decoder [Vaswani et al., 2017]

First, let's look at the Transformer Encoder and Decoder Blocks at a high level



The Transformer Encoder-Decoder [Vaswani et al., 2017]

Next, let's look at the Transformer Encoder and Decoder Blocks

What's left in a Transformer Encoder Block that we haven't covered?

1. **Key-query-value attention:** How do we get the k, q, v vectors from a single word embedding?
2. **Multi-headed attention**: Attend to multiple places in a single layer!
3. **Tricks to help with training!**
    1. Residual connections
    2. Layer normalization
    3. Scaling the dot product
    4. These tricks **don't improve** what the model is able to do; they help improve the training process. Both of these types of modeling improvements are very important!

The Transformer Encoder: Key-Query-Value Attention

- We saw that self-attention is when keys, queries, and values come from the same source. The Transformer does this in a particular way:
  - Let $x_1, \ldots, x_T$ be input vectors to the Transformer encoder; $x_i \in \mathbb{R}^d$

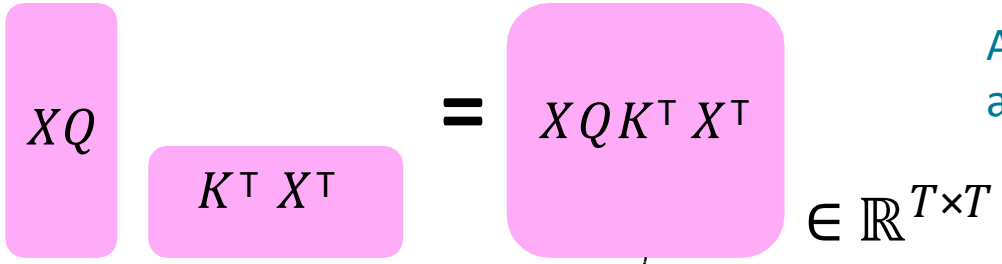
- Then keys, queries, values are:
  - $k_i = Kx_i$, where $K \in \mathbb{R}^{d \times d}$ is the key matrix.
  - $q_i = Qx_i$, where $\mathrm{Q} \in \mathbb{R}^{d \times d}$ is the query matrix.
  - $v_i = Vx_i$, where $\mathrm{V} \in \mathbb{R}^{d \times d}$ is the value matrix.

- These matrices allow *different aspects* of the x vectors to be used/emphasized in each of the three roles.

The Transformer Encoder: Key-Query-Value Attention

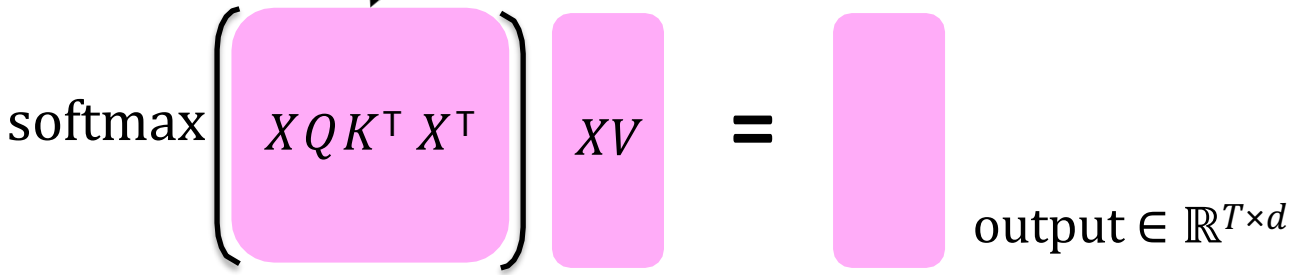
- Let's look at how key-query-value attention is computed, in matrices.
  - Let $X = [x_1; \ldots; x_T] \in \mathbb{R}^{T \times d}$ be the concatenation of input vectors.
  - First, note that $XK \in \mathbb{R}^{T \times d}$, $XQ \in \mathbb{R}^{T \times d}$, $XV \in \mathbb{R}^{T \times d}$.
  - The output is defined as $\text{output} = \text{softmax}(XQ(XK)^\top) \times XV$

First, take the query-key dot products in one matrix multiplication: $XQ\,(XK)^\top$



All pairs of attention scores!

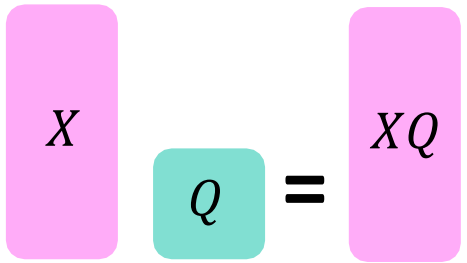
Next, softmax, and co mpute the weighted a verage with another matrix multiplication.



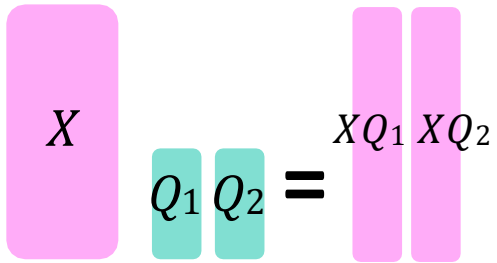
The Transformer Encoder: Multi-headed attention

- What if we want to look in multiple places in the sentence at once?
  - For word i, self-attention "looks" where $x^\top Q^\top K x_j$ is high, but maybe we want to focus on different j for different reasons?
- **We'll define multiple attention "heads" through multiple Q,K,V matrices**
- Let, $Q_l, K_l, V_l \in \mathbb{R}^{d \times \frac{d}{h}}$, where h is the number of attention heads, and l ranges from 1 to h.

Single-head attention
(just the query matrix)



Multi-head attention
(just two heads here)

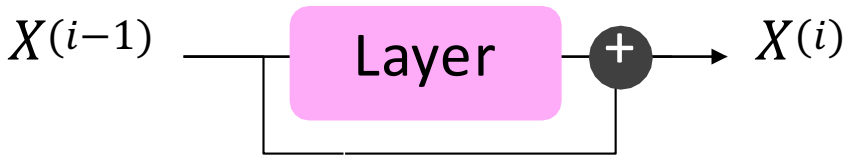


Same amount of computation as single-head self-attention!

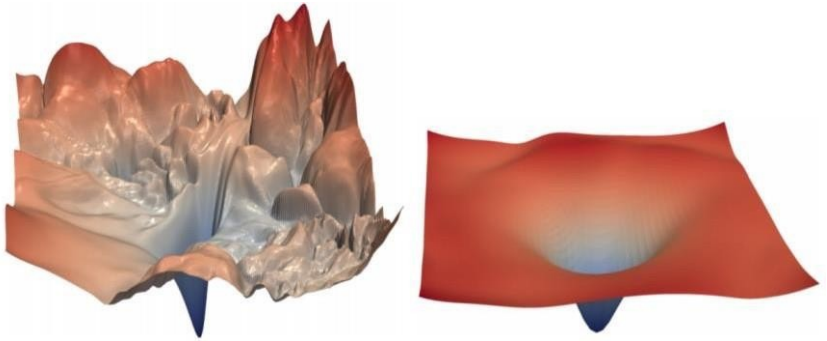
The Transformer Encoder: Residual connections [He et al., 2016]

- **Residual connections** are a trick to help models train better.
  - Instead of $X^{(i)} = \text{Layer}(X^{(i-1)})$ (where i represents the layer)

  - We let $X^{(i)} = X^{(i-1)} + \text{Layer}(X^{(i-1)})$ (so we only have to learn "the residual" from the previous layer)



  - Residual connections are thought to make the loss landscape considerably smoother (thus easier training!)



[no residuals] [residuals]

[Loss landscape visualization, Li et al., 2018, on a ResNet]

The Transformer Encoder: Layer normalization [Ba et al., 2016]

- **Layer normalization** is a trick to help models train faster.
- Idea: cut down on uninformative variation in hidden vector values by normaliz ing to unit mean and standard deviation **within each layer**.
  - LayerNorm's success may be due to its normalizing gradients [Xu et al., 2019]
- Let $x \in \mathbb{R}^d$ be an individual (word) vector in the model.
- Let $\mu = \sum_{j=1}^{d} x_j$; this is the mean; $\mu \in \mathbb{R}$.
- Let $\sigma = \sqrt{\frac{1}{d}\sum_{j=1}^{d}(x_j - \mu)^2}$; this is the standard deviation; $\sigma \in \mathbb{R}$.
- Let $\gamma \in \mathbb{R}^d$ and $\beta \in \mathbb{R}^d$ be learned "gain" and "bias" parameters. (Can omit!)
- Then layer normalization computes:

$$\text{output} = \frac{x - \mu}{\sqrt{\sigma + \epsilon}} * \gamma + \beta$$

Normalize by scalar mean and variance

Modulate by learned elementwise gain and bias

The Transformer Encoder: Scaled Dot Product [Vaswani et al., 2017]

- **"Scaled Dot Product"** attention is a final variation to aid in Transformer training.
- When dimensionality d becomes large, dot products between vectors tend to become large.
  - Because of this, inputs to the softmax function can be large, making the gradients small.
- Instead of the self-attention function we've seen:

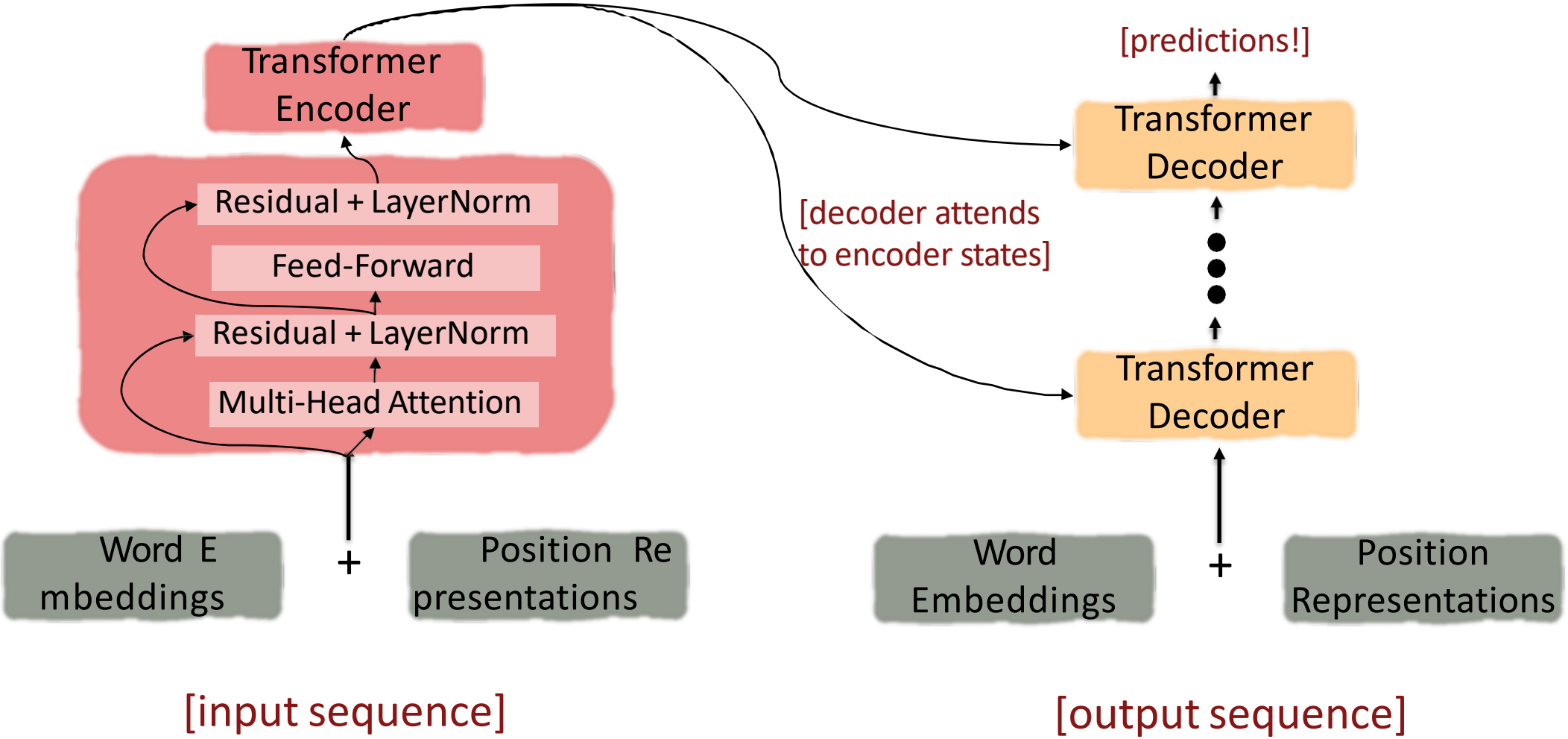
$$\text{output}_l = \text{softmax}\left(XQ_lK_l^\top X^\top\right)XV_l$$

- We divide the attention scores by $\sqrt{d/h}$, to stop the scores from becoming large just as a function of d/h (The dimensionality divided by the number of heads.)

$$\text{output}_l = \text{softmax}\left(\frac{XQ_lK_l^\top X^\top}{\sqrt{d/h}}\right)XV_l$$

The Transformer Encoder-Decoder [Vaswani et al., 2017]

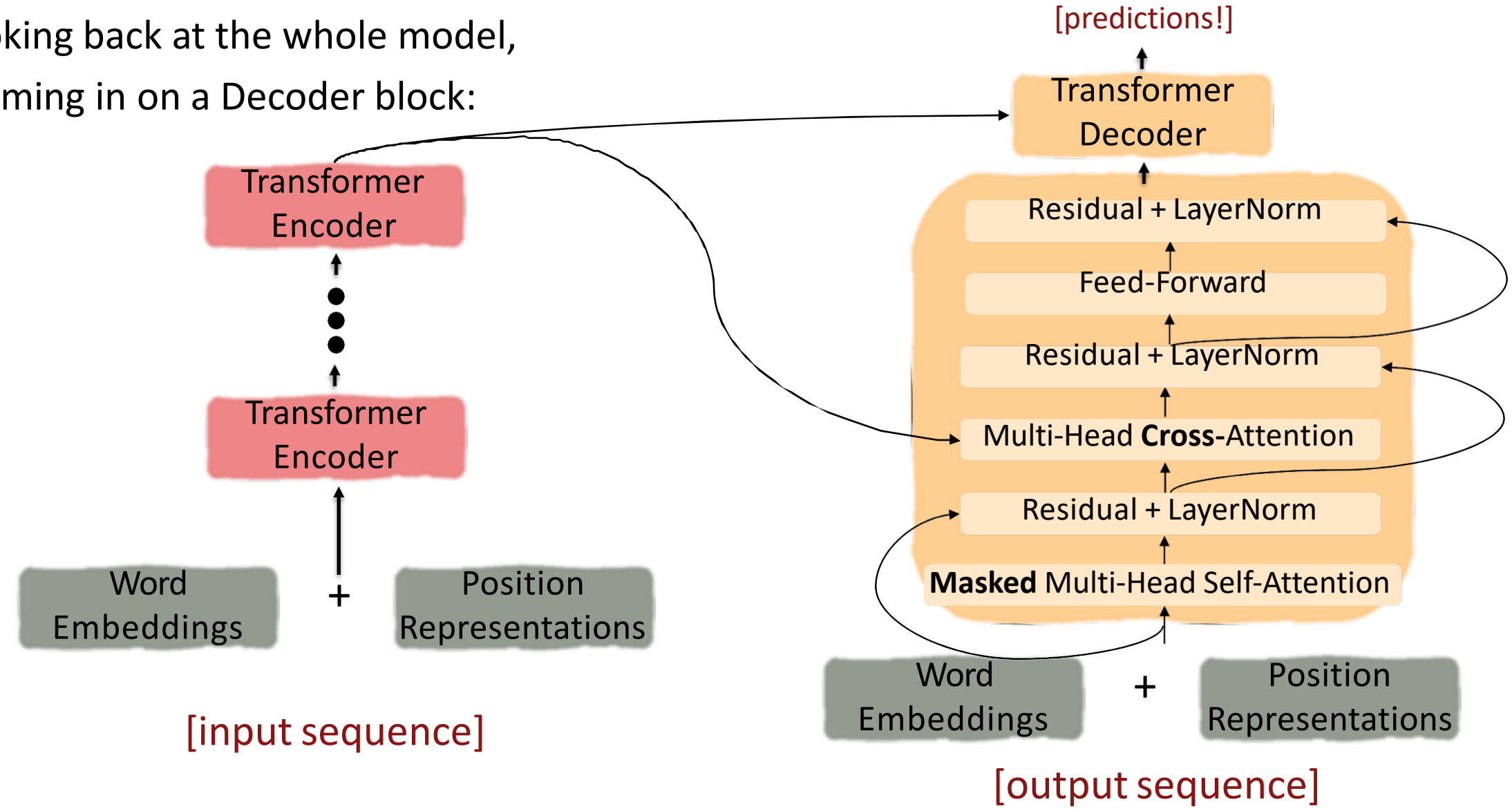
Looking back at the whole model, zooming in on an Encoder block:



The Transformer Encoder-Decoder [Vaswani et al., 2017]

Looking back at the whole model,

zooming in on a Decoder block:



The Transformer Decoder: Cross-attention (details)

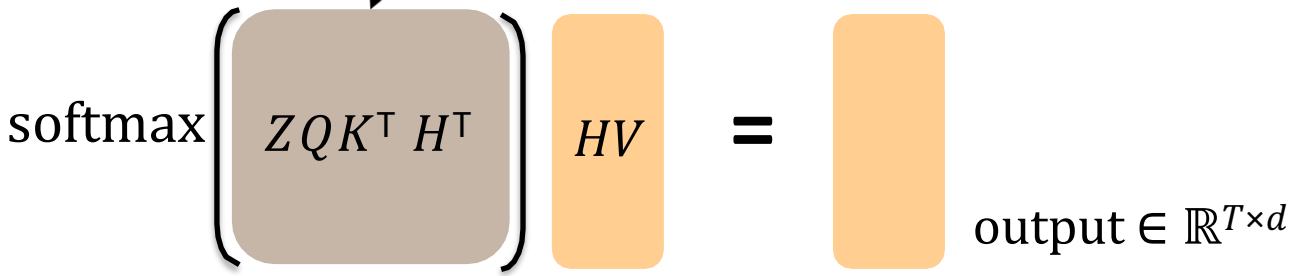
- We saw that self-attention is when keys, queries, and values come from the same source.
- In the decoder, we have attention that looks more like what we saw last week.
- Let $h_1, \ldots, h_T$ be **output** vectors **from** the Transformer **encoder**; $x_i \in \mathbb{R}^d$
- Let $z_1, \ldots, z_T$ be input vectors from the Transformer **decoder**, $z_i \in \mathbb{R}^d$
- Then keys and values are drawn from the **encoder** (like a memory):
  - $k_i = Kh_i$, $v_i = Vh_i$.
- And the queries are drawn from the **decoder**, $q_i = Qz_i$.

The Transformer Decoder: Cross-attention (details)

- Let's look at how cross-attention is computed, in matrices.
  - Let $\mathrm{H} = [h_1; \ldots; h_T] \in \mathbb{R}^{T \times d}$ be the concatenation of encoder vectors.
  - Let $\mathrm{Z} = [z_1; \ldots; z_T] \in \mathbb{R}^{T \times d}$ be the concatenation of decoder vectors.
  - The output is defined as $\text{output} = \text{softmax}(ZQ(HK)^\top) \times HV$.

First, take the query-key dot products in one matrix multiplication: $ZQ \quad (HK)^\top$

Next, softmax, and compute the weighted average with another matrix multiplication.



Quadratic computation as a function of sequence length

- One of the benefits of self-attention over recurrence was that it's highly parallelizable.
- However, its total number of operations grows as $O\ (T^2 d)$, where T is the sequence length, and d is the dimensionality.

$$XQ \quad K^\top X^\top = XQK^\top X^\top \in \mathbb{R}^{T \times T}$$

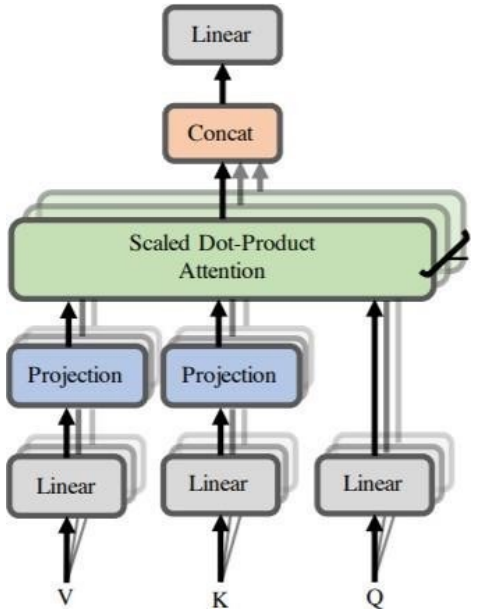
Need to compute all pairs of interactions!
$O(T^2 d)$

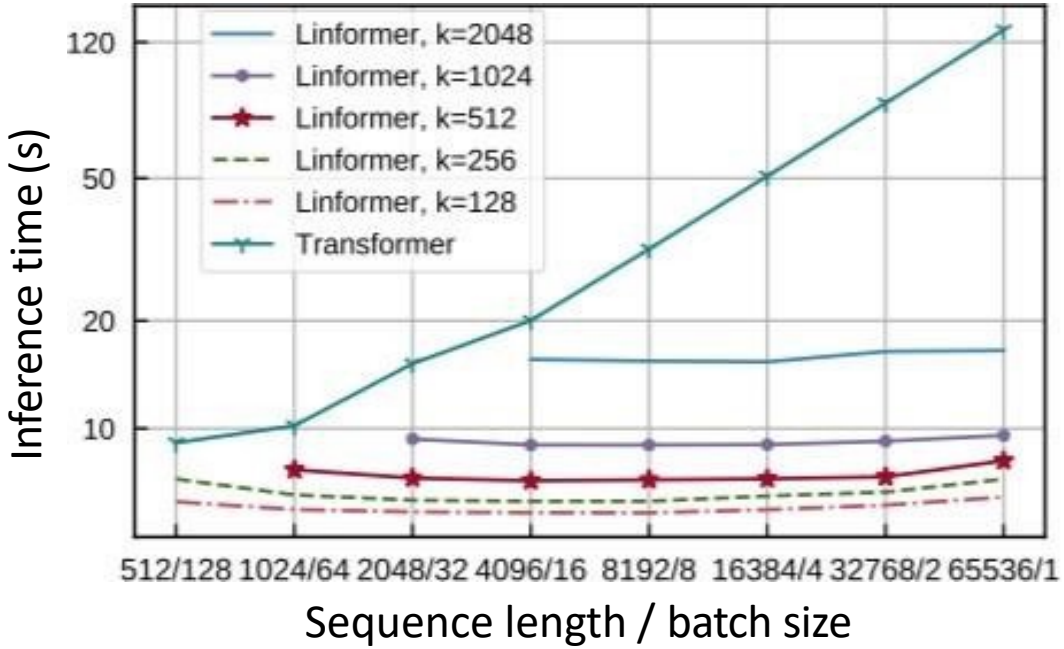
- Think of d as around $\mathbf{1,000}$.
  - So, for a single (shortish) sentence, $T \leq 30; T^2 \leq \mathbf{900}$.
  - In practice, we set a bound like $T = 512$.
  - **But what if we'd like $T \geq \mathbf{10,000}$?** For example, to work on long documents?

Recent work on improving on quadratic self-attention cost

- Considerable recent work has gone into the question, *Can we build models like Transformers without paying the* $O(T^2)$ *all-pairs self-attention cost?*
- For example, **Linformer** [Wang et al., 2020]

Key idea: map the sequence length dimension to a lower-dimensional space for values, keys

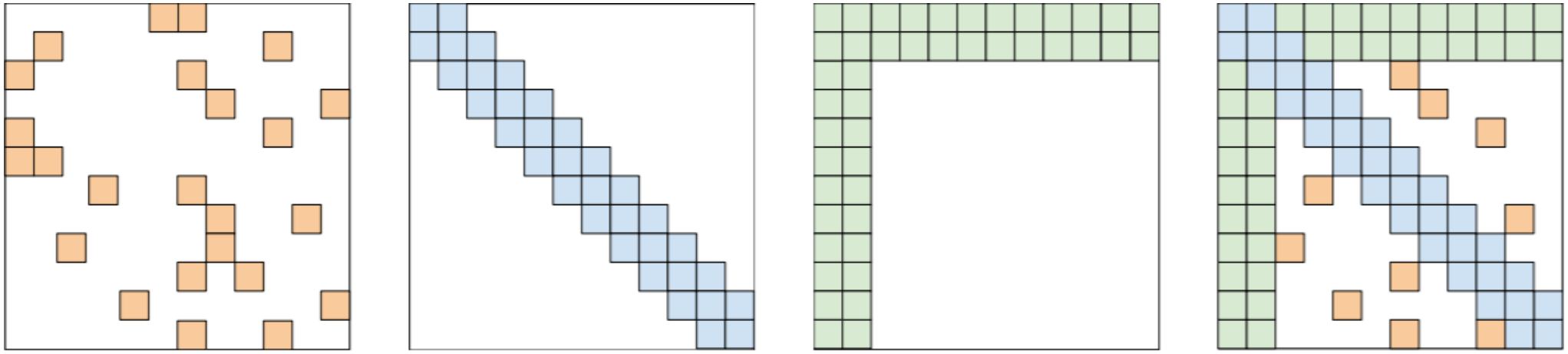




Recent work on improving on quadratic self-attention cost

- Considerable recent work has gone into the question, *Can we build models like Transformers without paying the $O(T^2)$ all-pairs self-attention cost?*
- For example, **BigBird** [Zaheer et al., 2021]

Key idea: replace all-pairs interactions with a family of other interactions, **like local windows**, **looking at everything**, and **random interactions**.



(a) Random attention (b) Window attention (c) Global Attention (d) BIGBIRD

Thank you!
Q & A