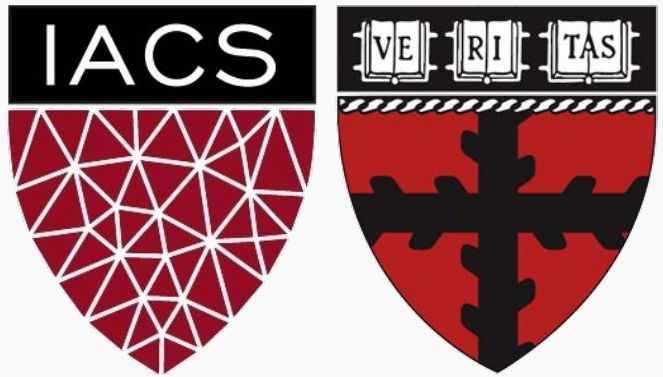
Lecture 17: Language Modelling 2

CS109B Data Science 2

Pavlos Protopapas, Mark Glickman, and Chris Tanner



Outline

- Seq2Seq +Attention
- Transformers +BERT
- Embeddings

Embedding of "stick" in "Let's stick to" - Step #2

1- Concatenate hidden layers

2- Multiply each vector by a weight based on the task

X s_2

X s_1

X s_0

3- Sum the (now weighted) vectors

ELMo embedding of "stick" for this task in this context

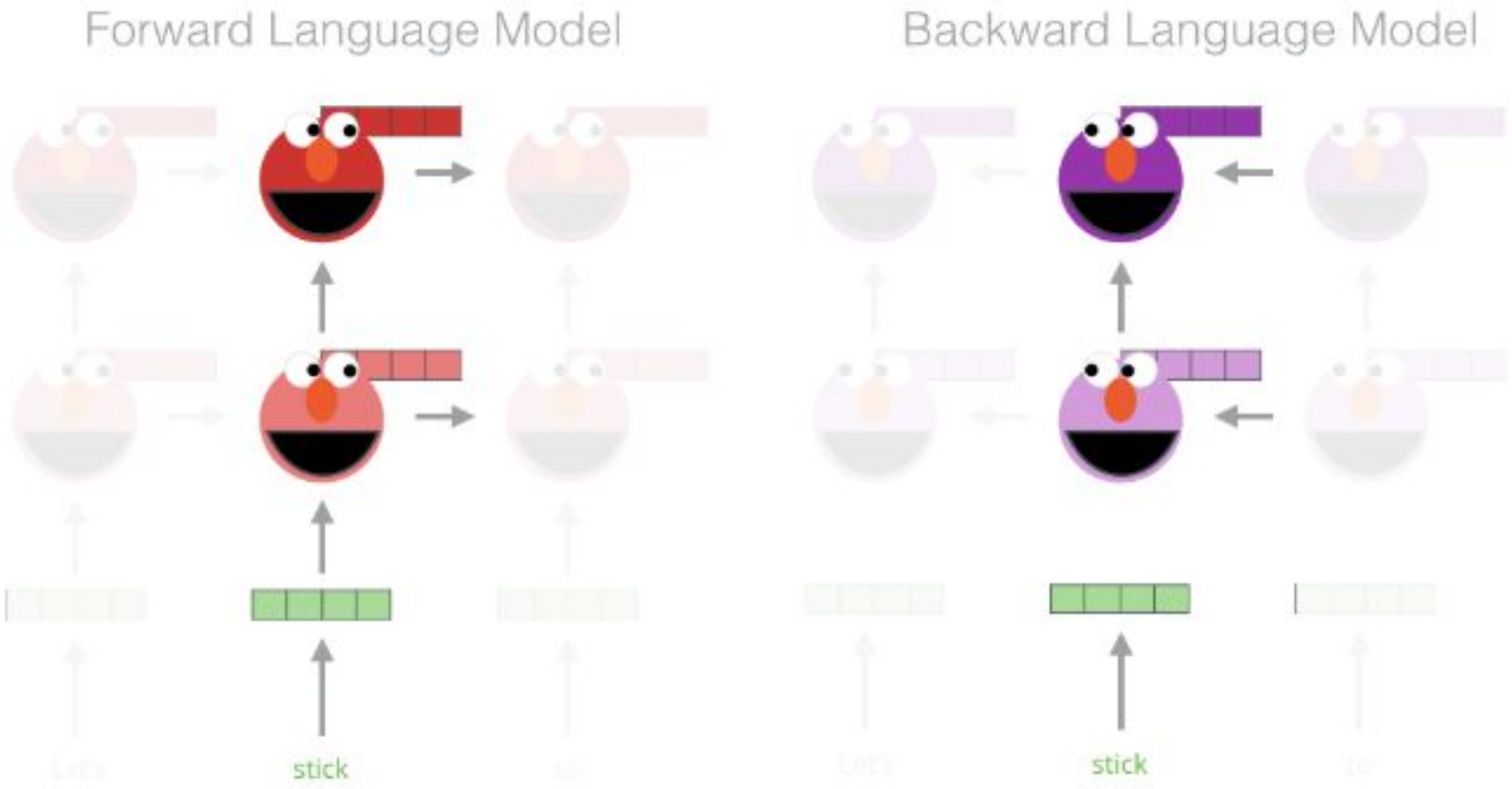


Illustration: http://jalammar.github.io/illustrated-bert/

ELMo: **Stacked Bi-directional LSTMs**

- ELMo yielded incredibly good word embeddings, which yielded state-of-the-art results when applied to many NLP tasks.
- Main ELMo takeaway: given enough training data, having tons of explicit connections between your vectors is useful (system can determine how to best use context)

ELMo Slides: https://www.slideshare.net/shuntaroy/a-review-of-deep-contextualized-word-representations-peters-2018

REFLECTION

So far, for all of our sequential modelling, we have been concerned with emitting 1 output per input datum.

Sometimes, a *sequence* is the smallest granularity we care about though (e.g., an English sentence)


WAS THAT...
SARCASM?

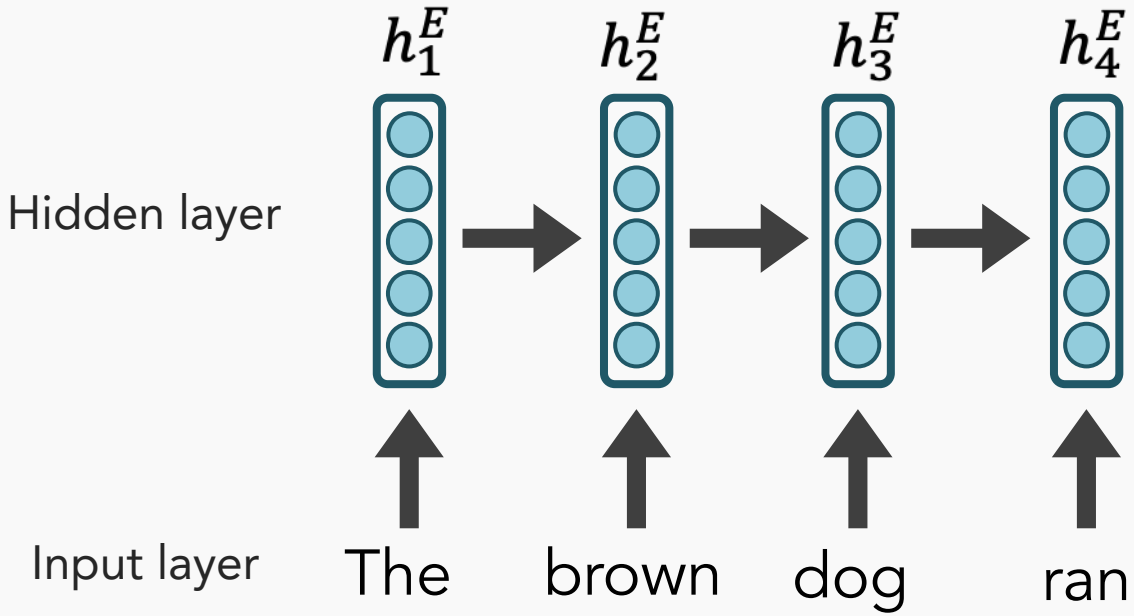
Outline

- **Seq2Seq +Attention**
- Transformers +BERT
- Embeddings

Sequence-to-Sequence (seq2seq)

- If our input is a sentence in Language A, and we wish to translate it to Language B, it is clearly sub-optimal to translate word by word (like our current models are suited to do).
- Instead, let a ***sequence*** of tokens be the unit that we ultimately wish to work with (a sequence of length **N** may emit a sequences of length **M**)
- Seq2seq models are comprised of **2 RNNs**: 1 encoder, 1 decoder

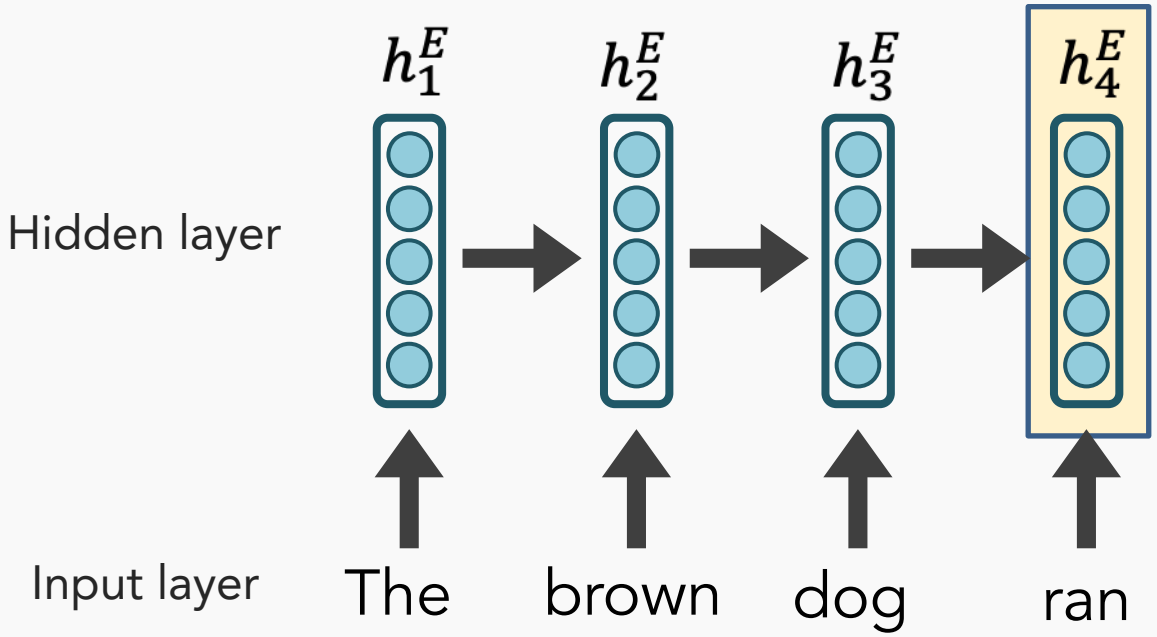
Sequence-to-Sequence (seq2seq)



ENCODER RNN

Sequence-to-Sequence (seq2seq)

The final hidden state of the encoder RNN
is the initial state of the decoder RNN



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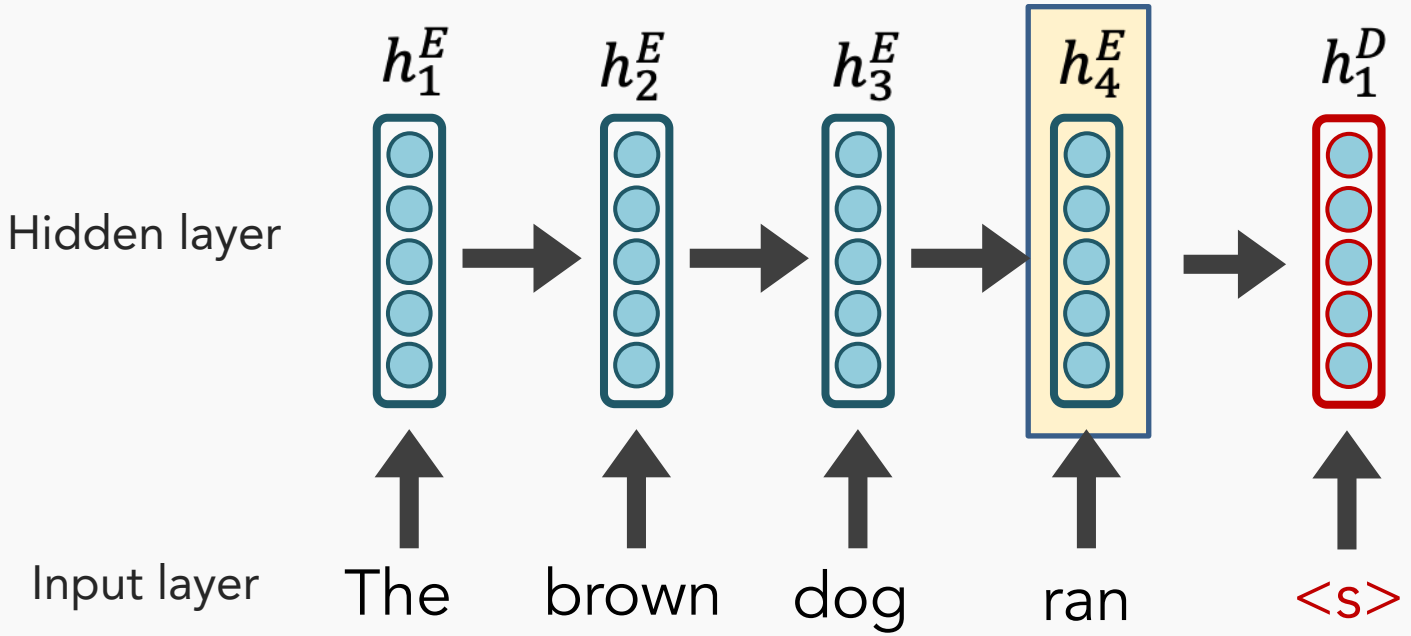

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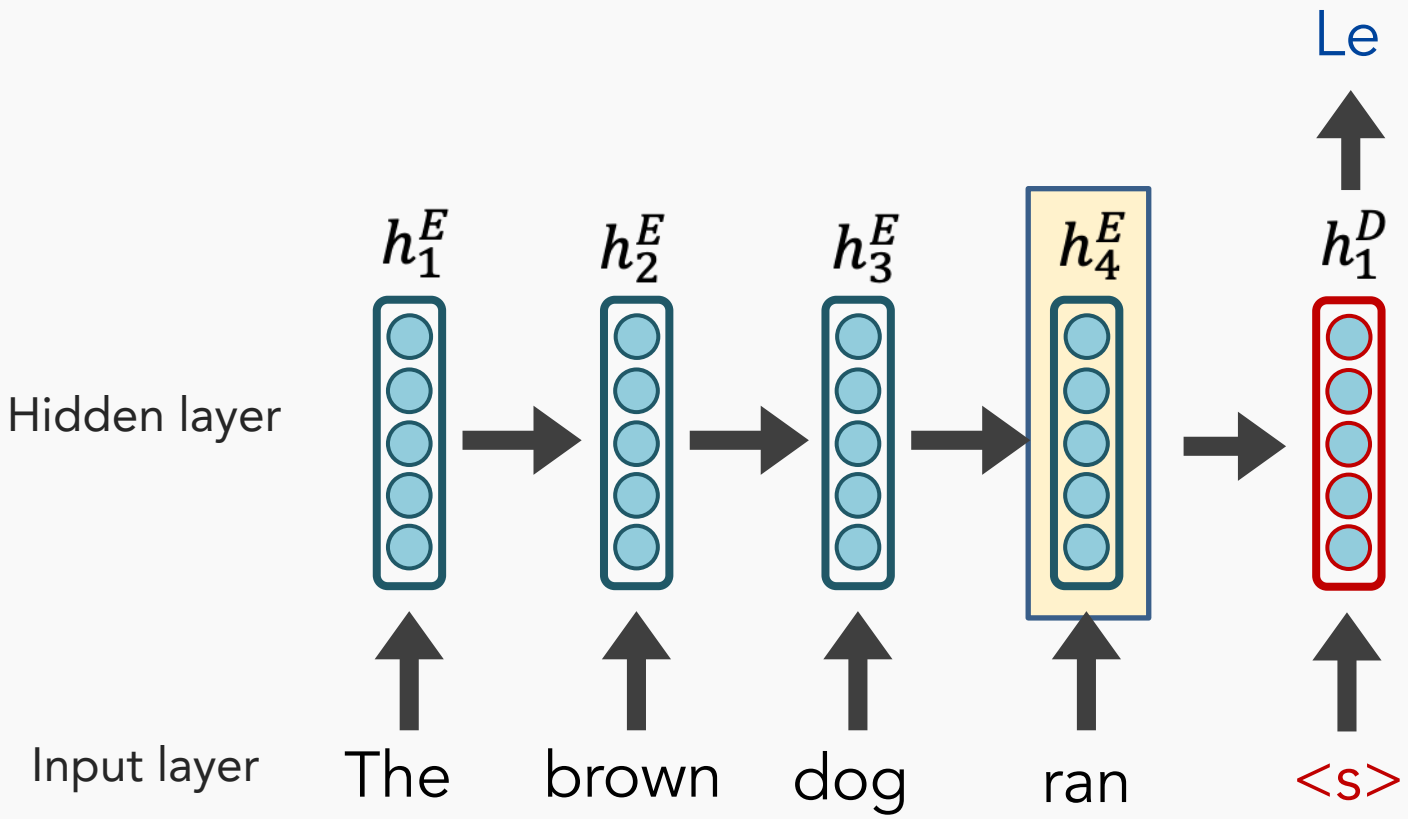

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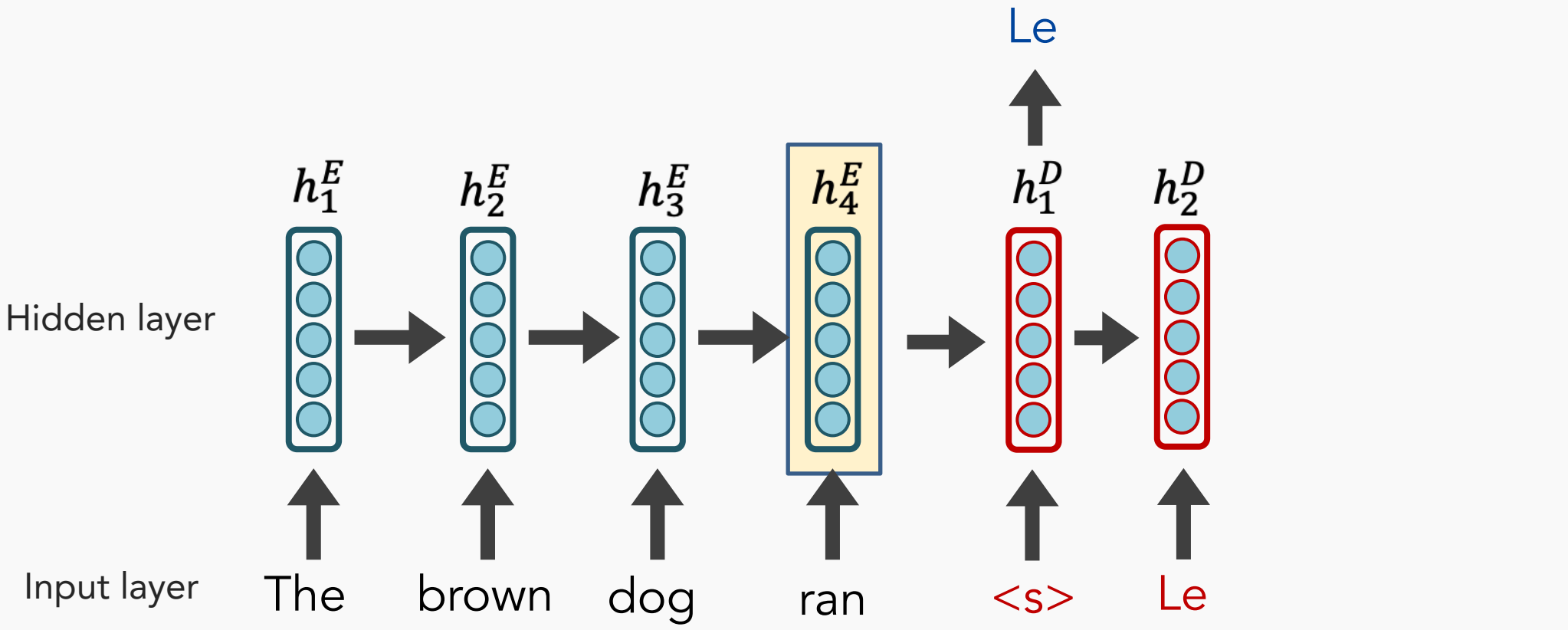

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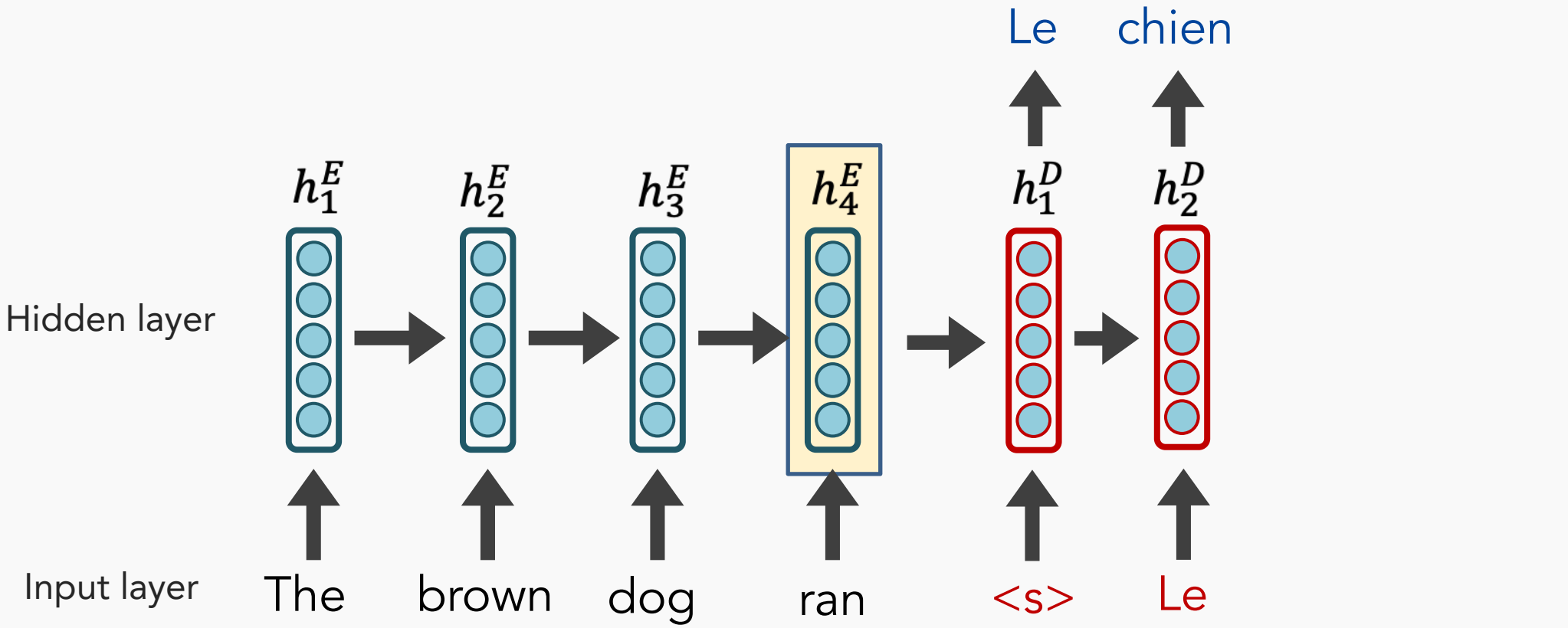

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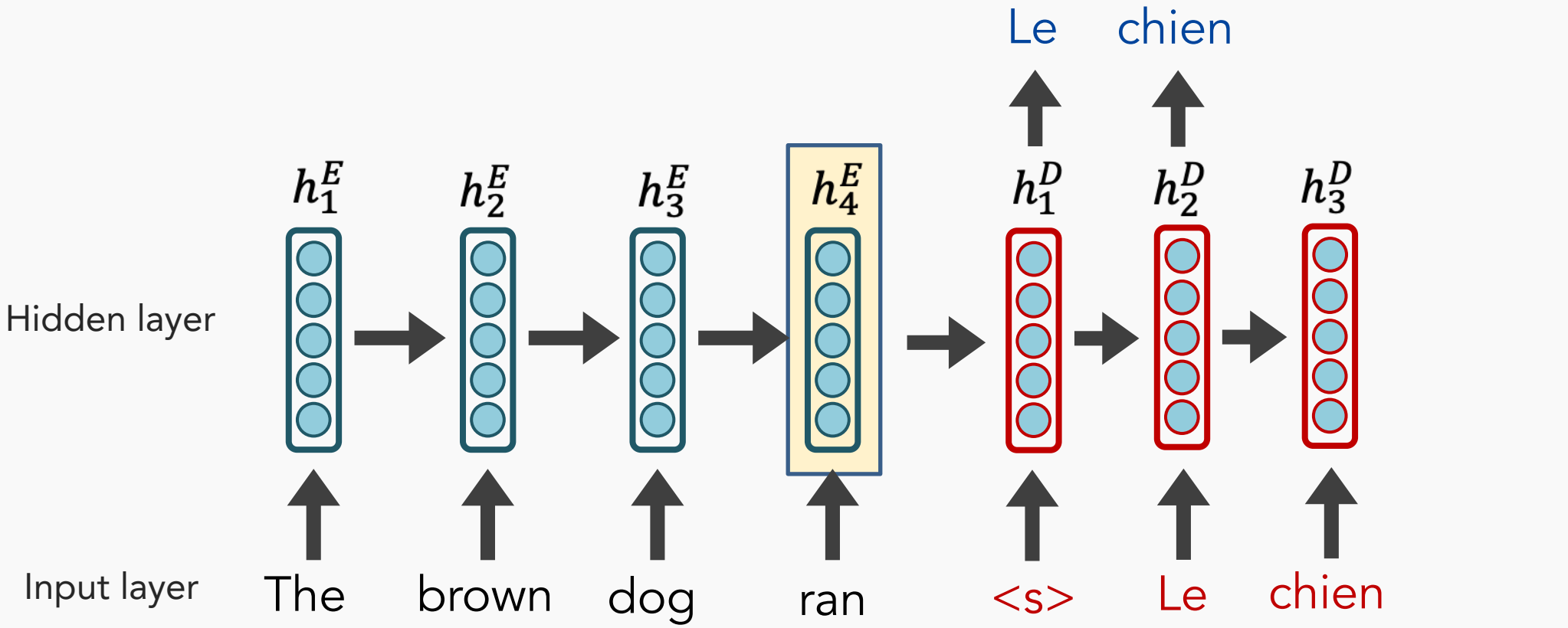

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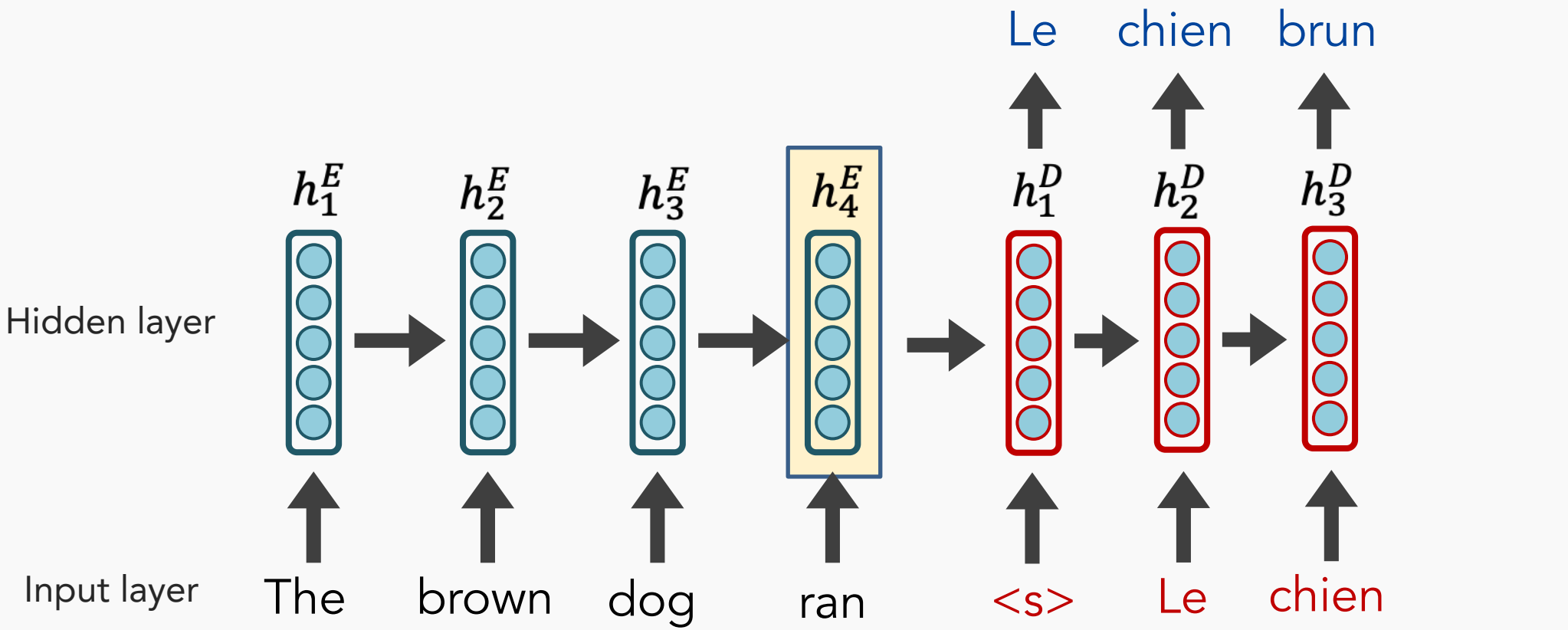

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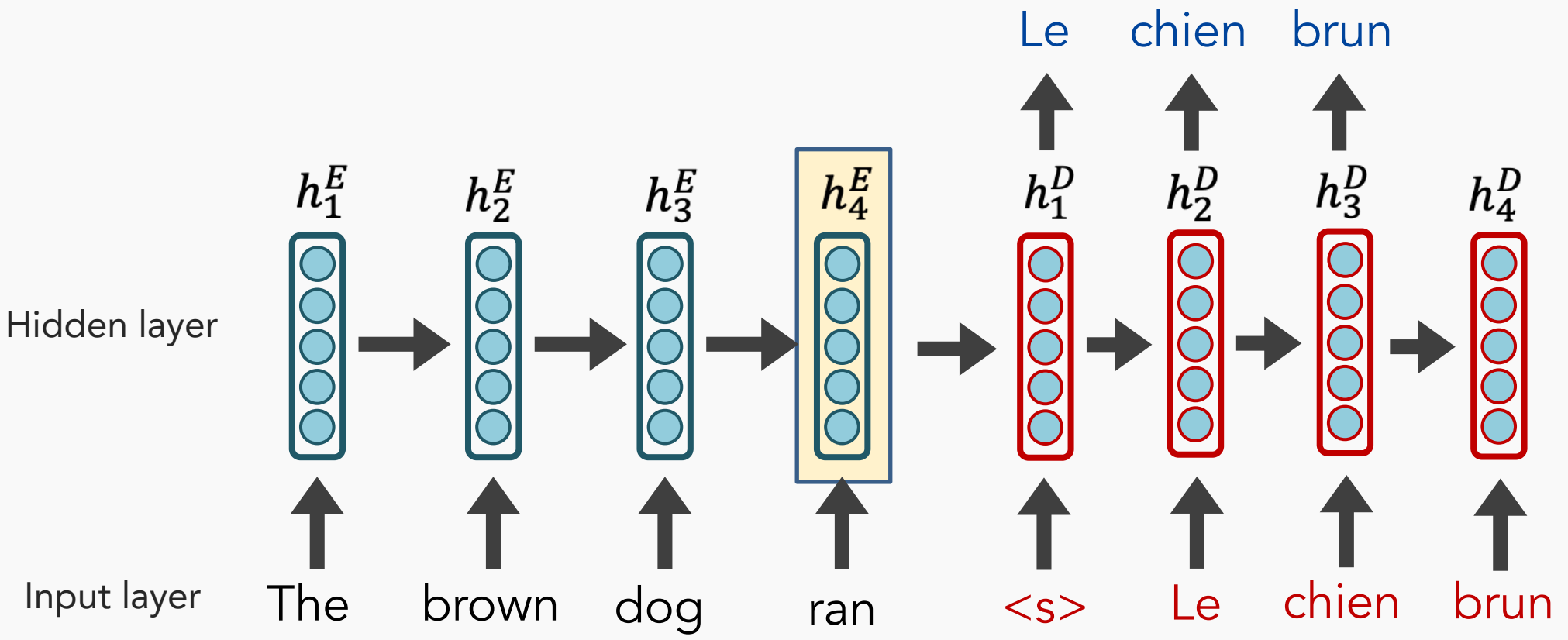

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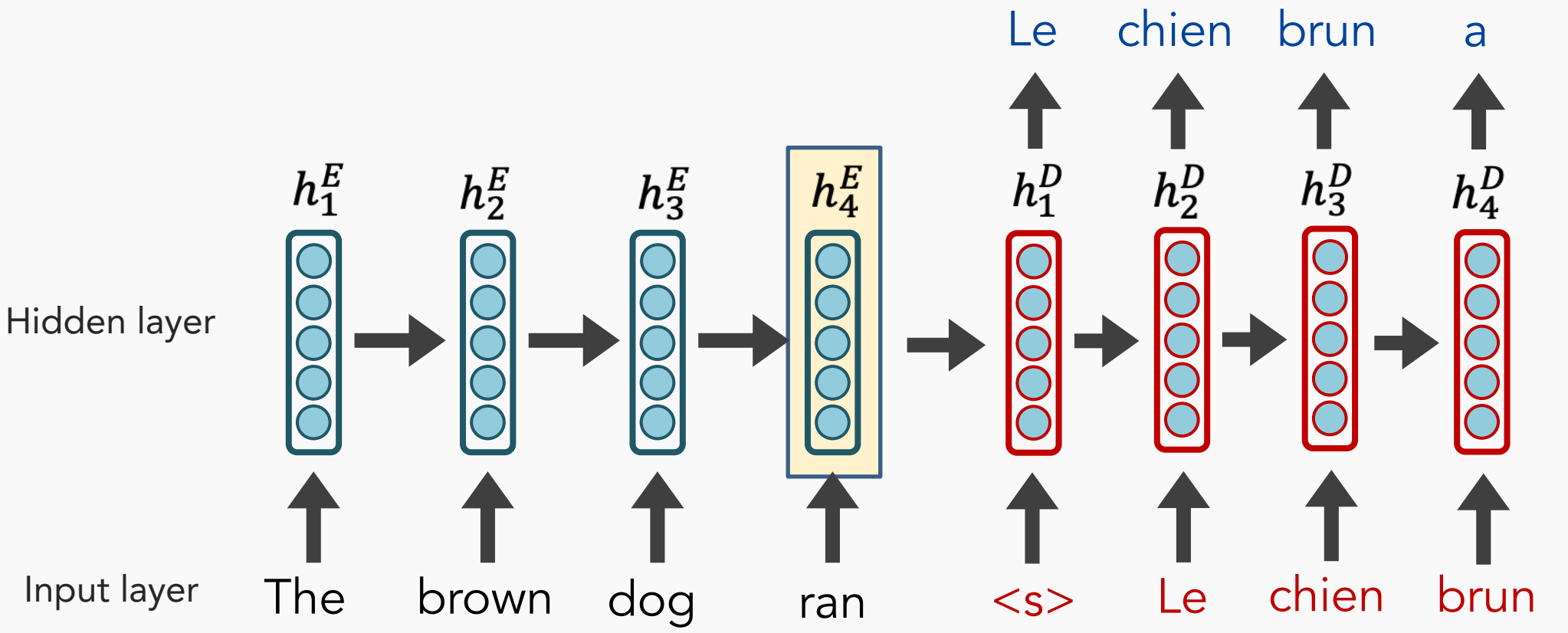

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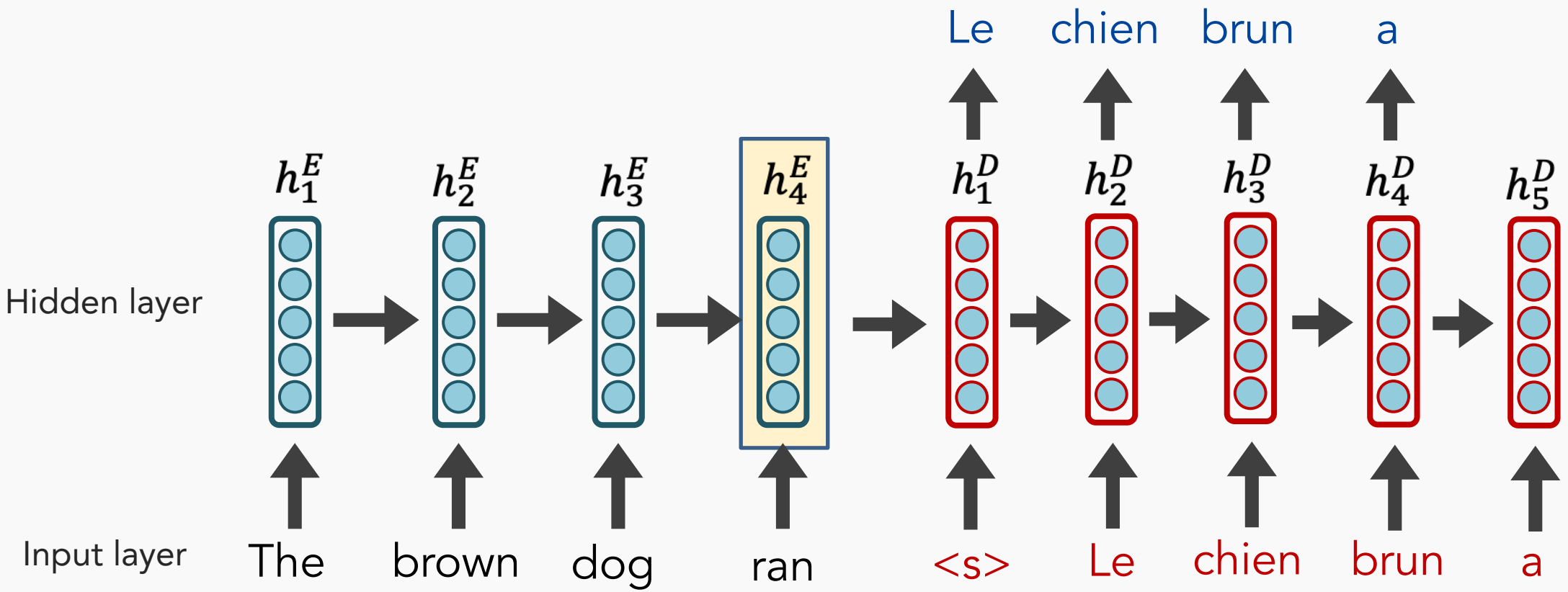

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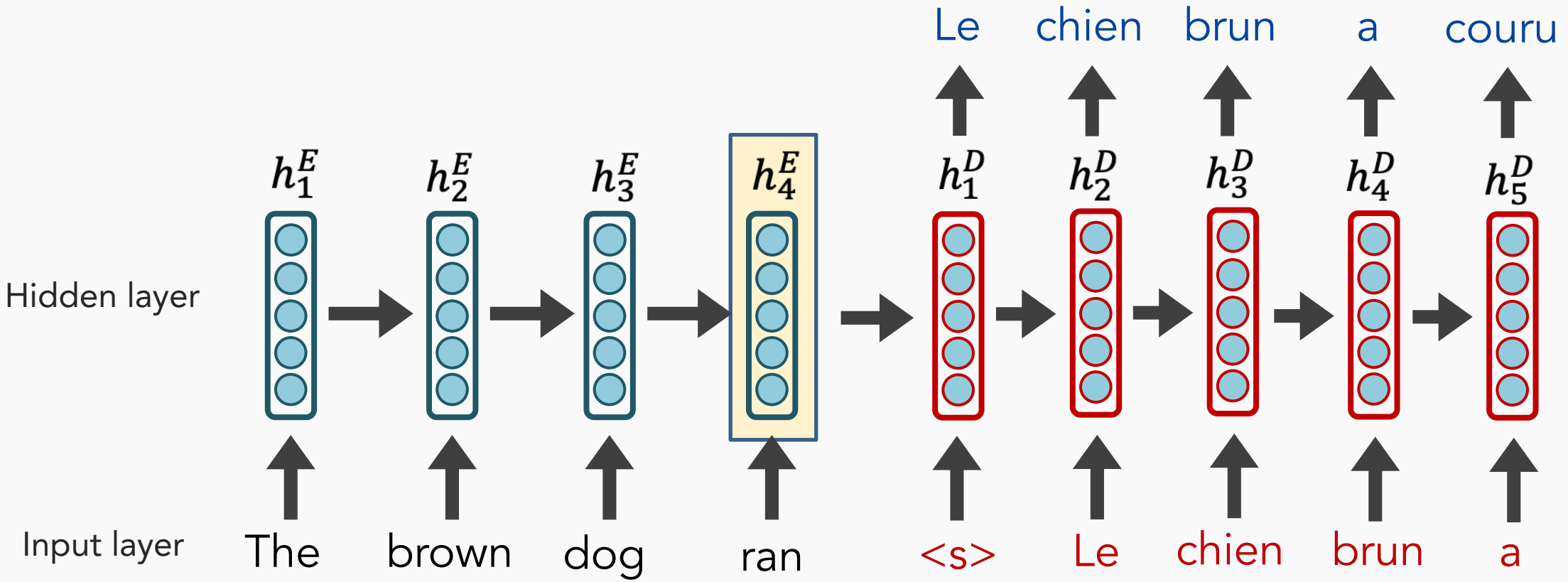

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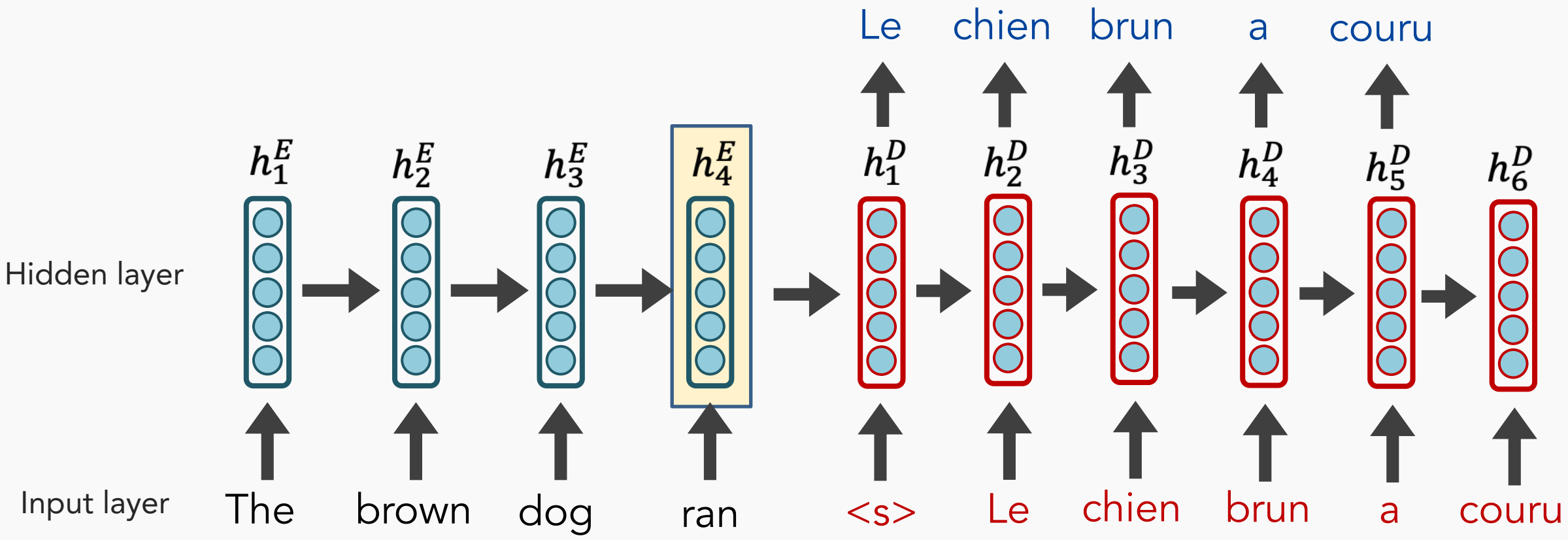

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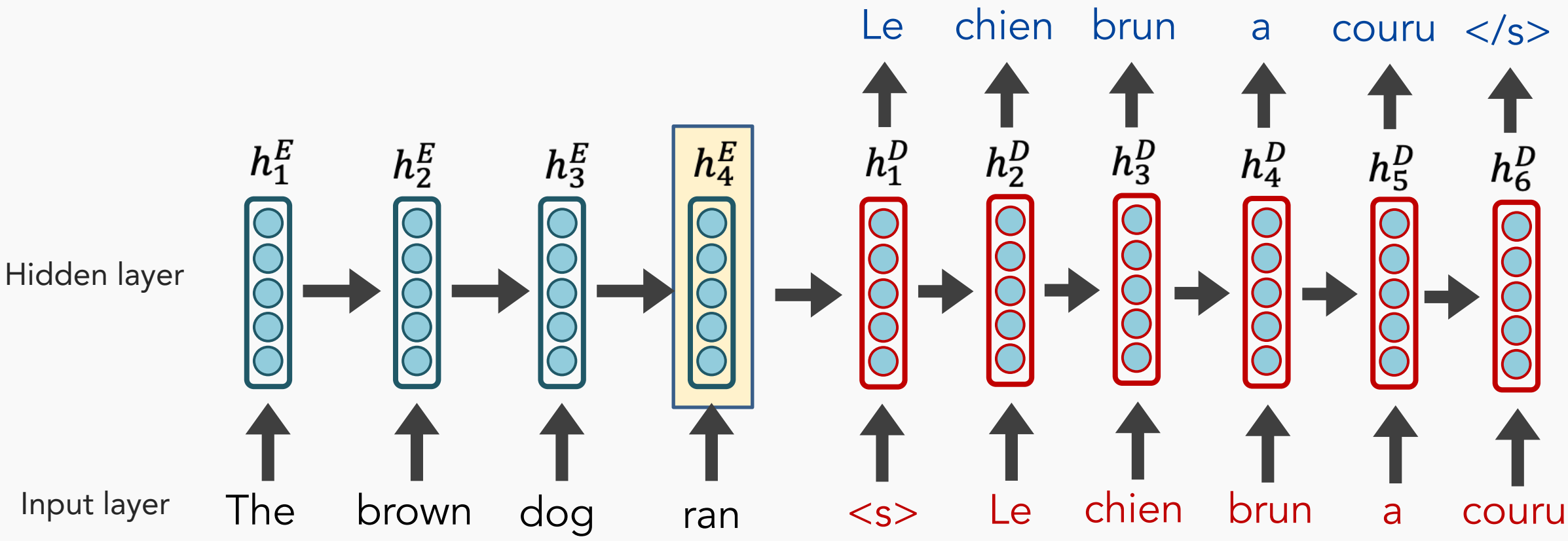

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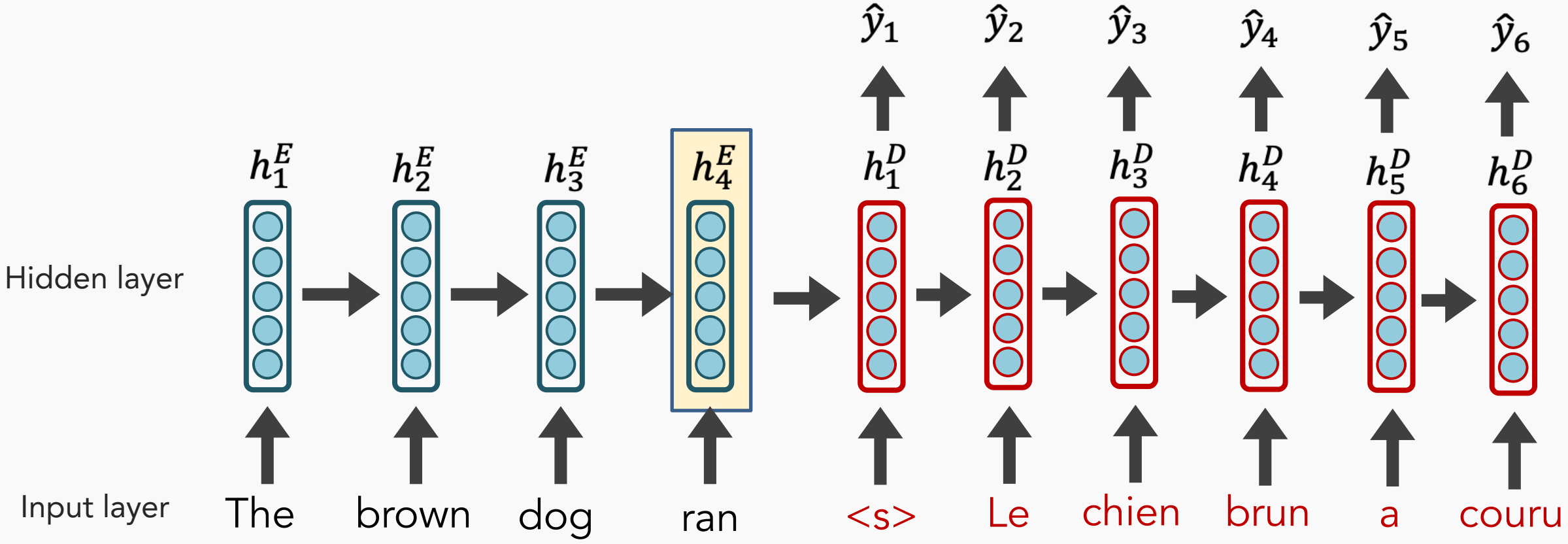

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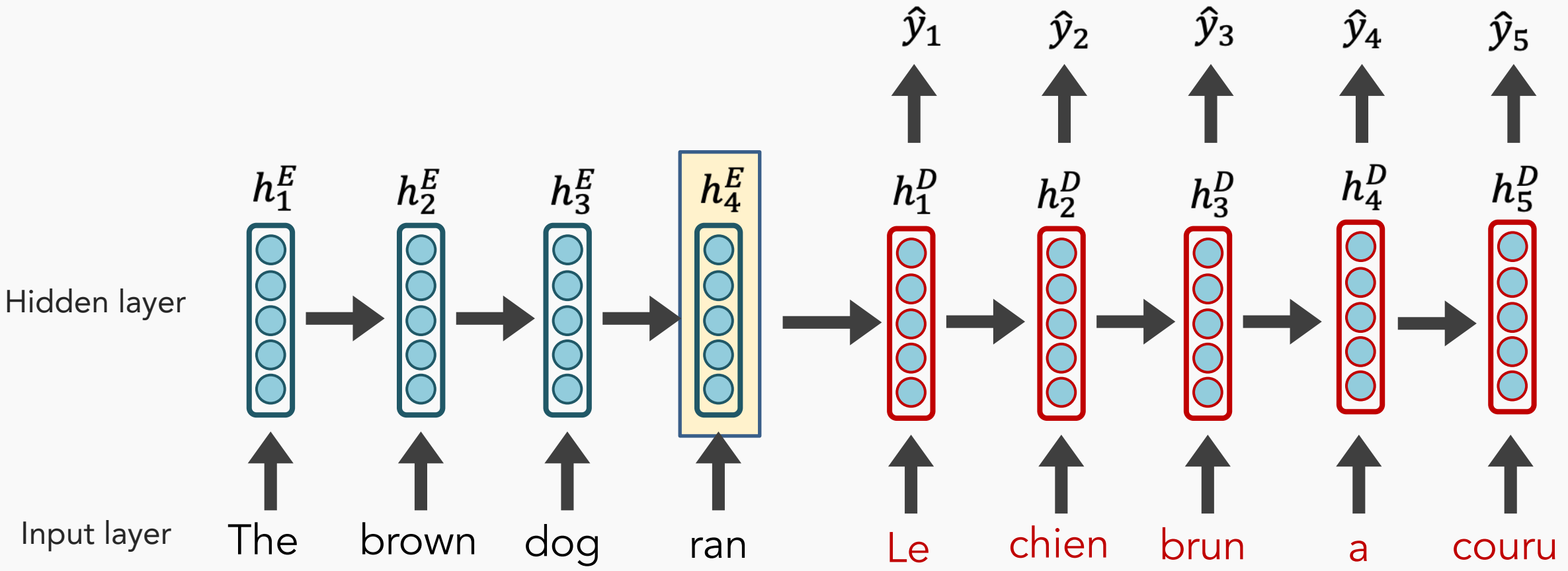
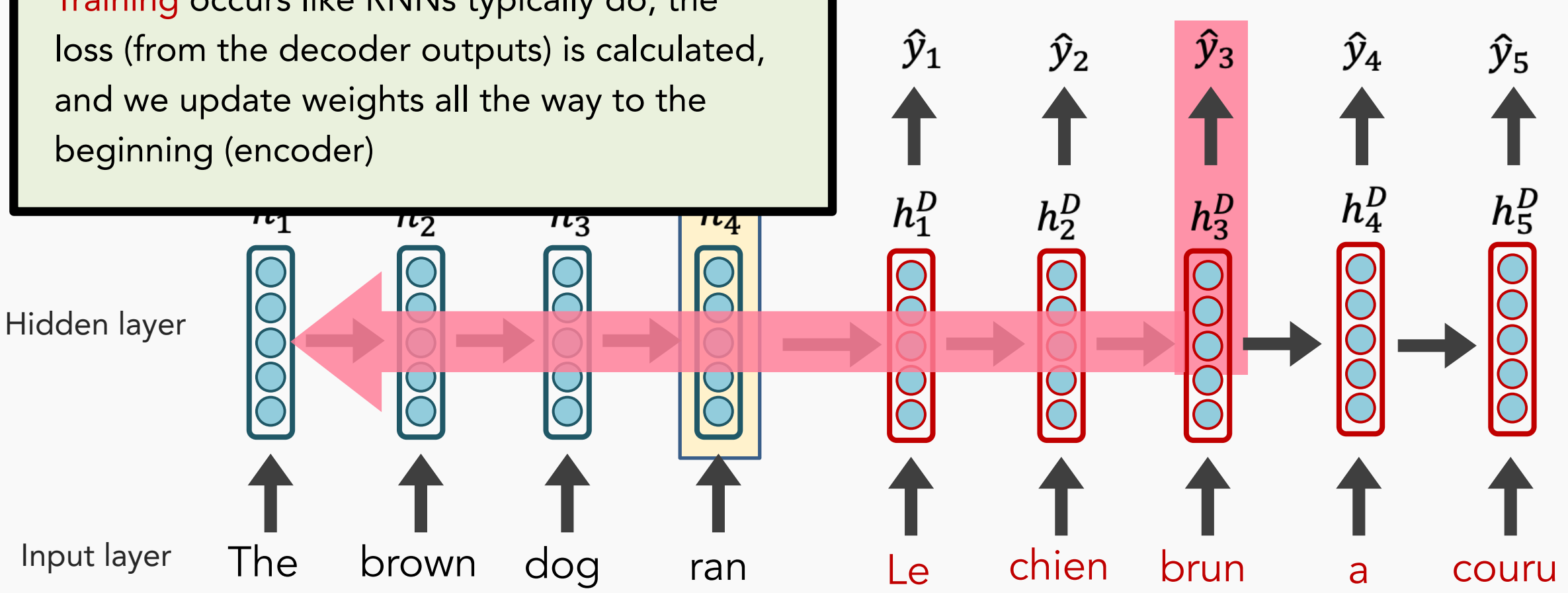


Sequence-to-Sequence (seq2seq)

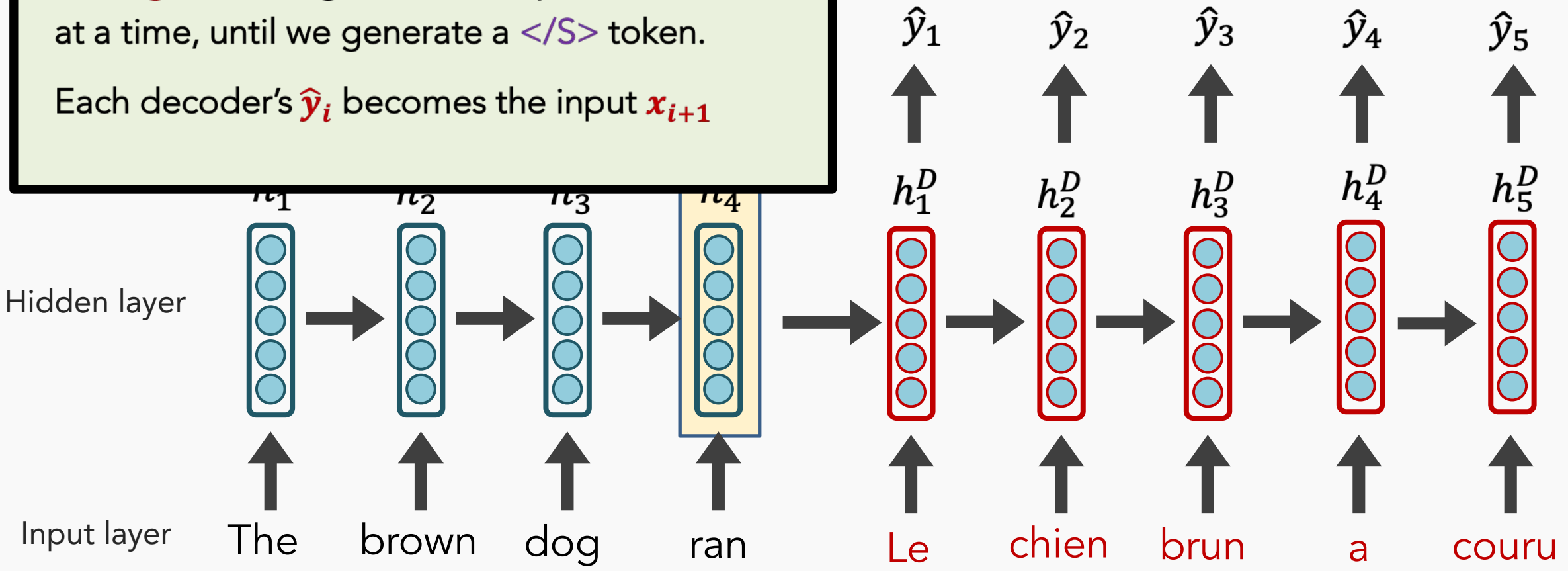
Training occurs like RNNs typically do; the loss (from the decoder outputs) is calculated, and we update weights all the way to the beginning (encoder)



Sequence-to-Sequence (seq2seq)

Testing decoder generates outputs one word at a time, until we generate a </S> token.

Each decoder's $\hat{y}_i$ becomes the input x_{i+1}



ENCODER RNN

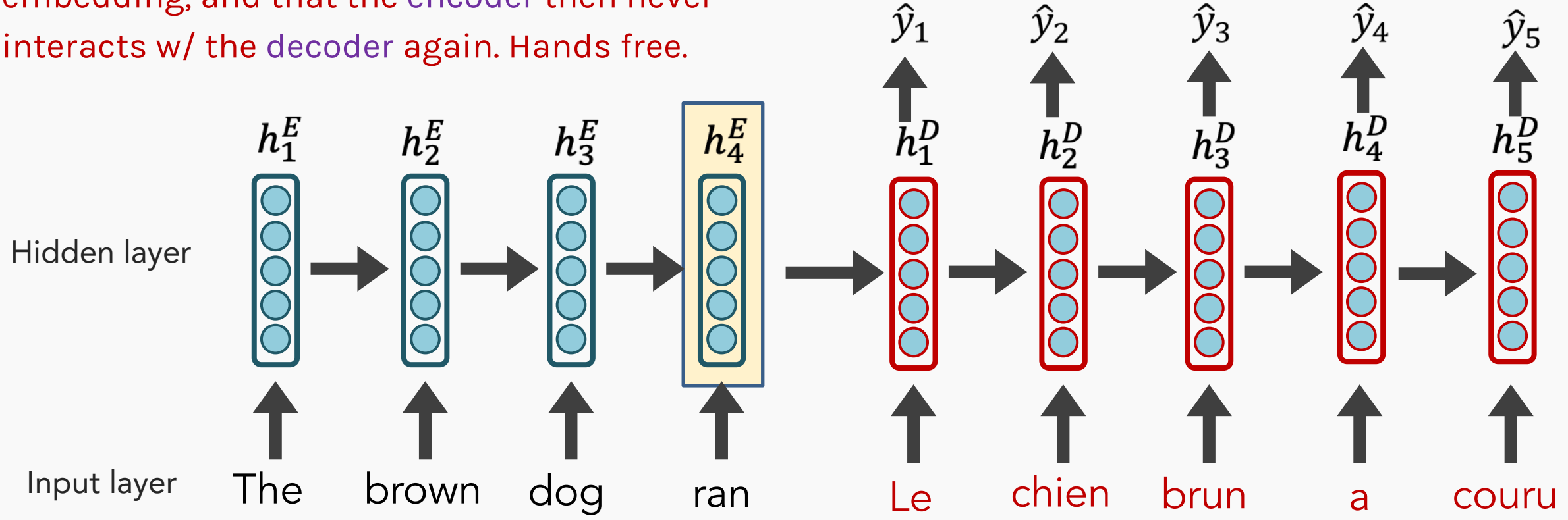
DECODER RNN

Sequence-to-Sequence (seq2seq)

See any issues with this traditional **seq2seq** paradigm?

Sequence-to-Sequence (seq2seq)

It's crazy that the entire "meaning" of the 1st sequence is expected to be packed into this one embedding, and that the encoder then never interacts w/ the decoder again. Hands free.

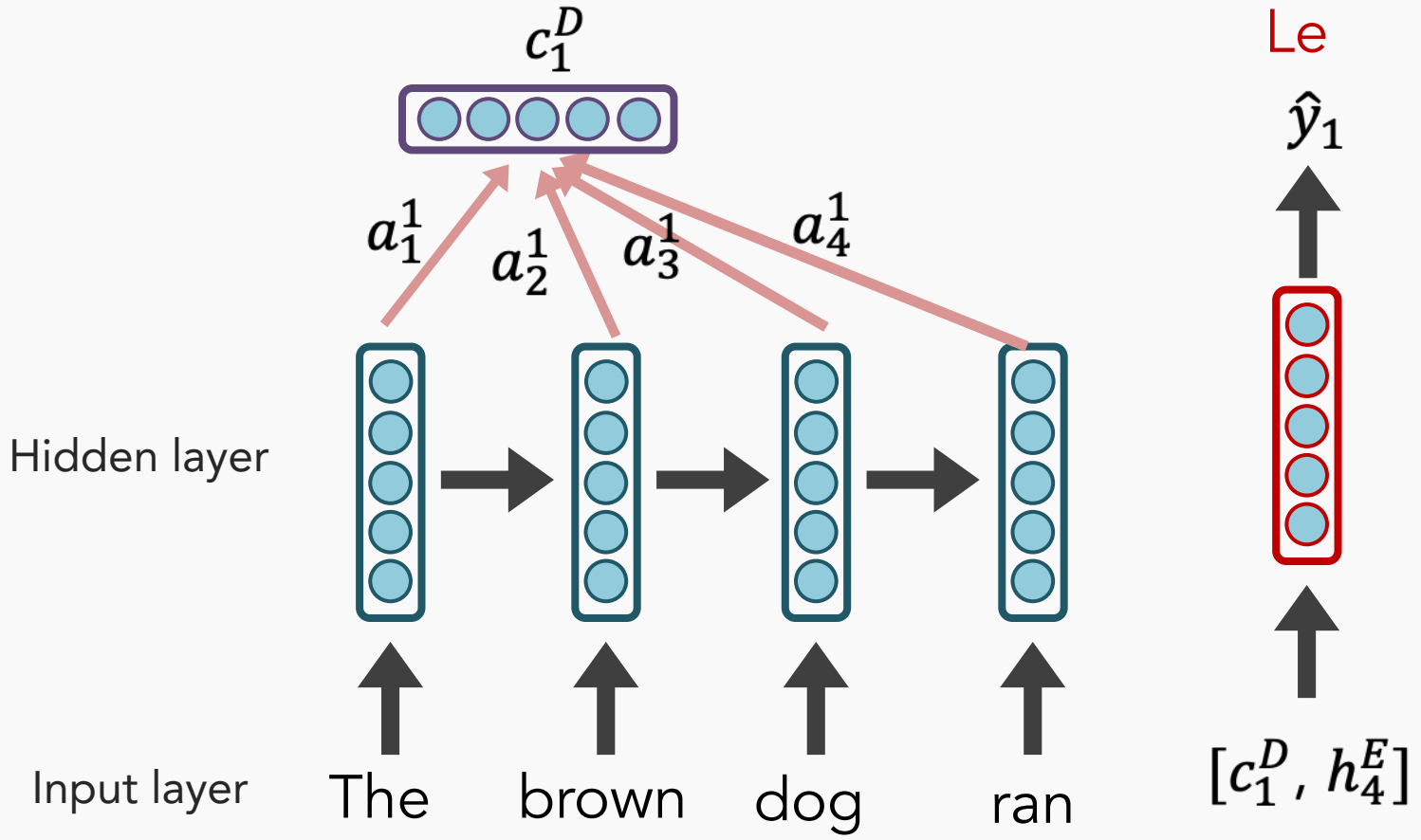


Sequence-to-Sequence (seq2seq)

Instead, what if the decoder, at each step, pays attention to a *distribution* of all of the encoder's hidden states?

seq2seq + Attention

NOTE: each attention weight a_i^j is based on the decoder's current hidden state, too.



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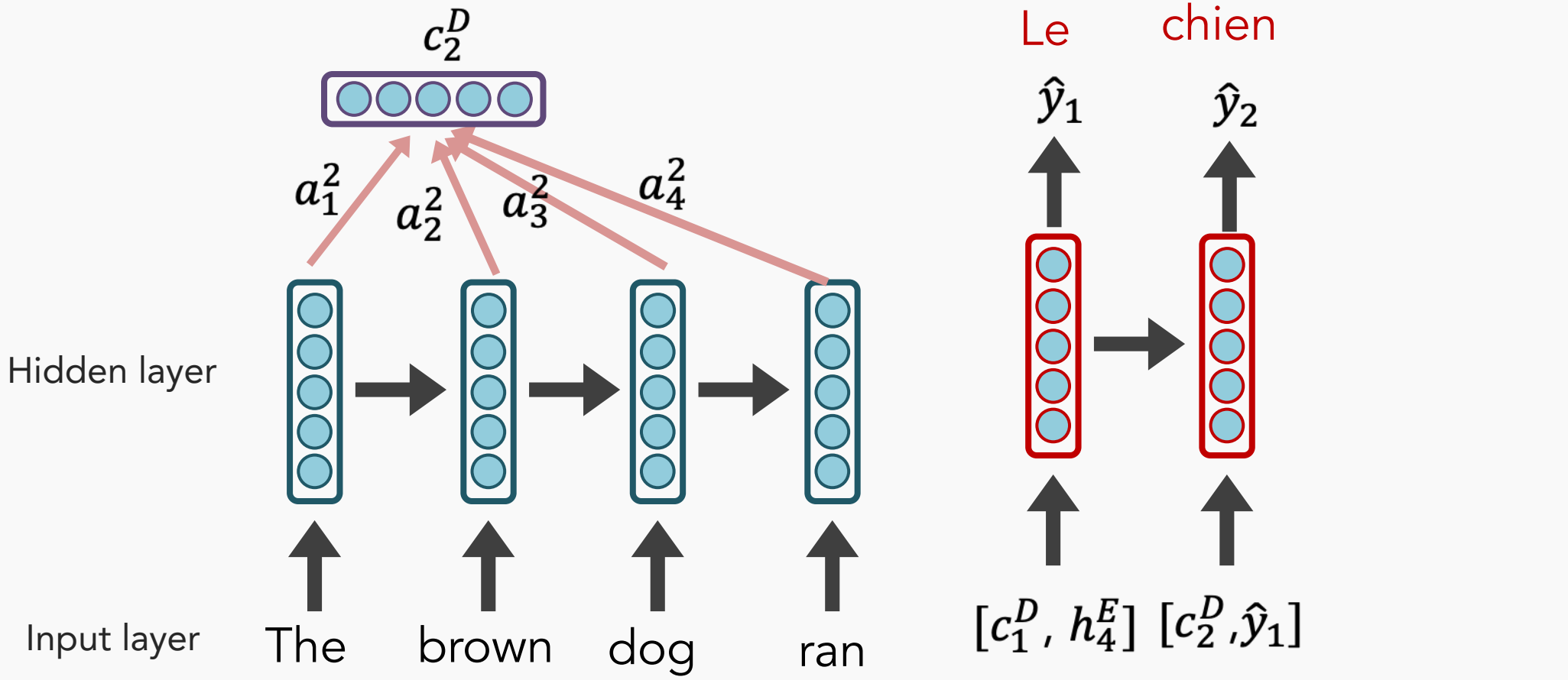

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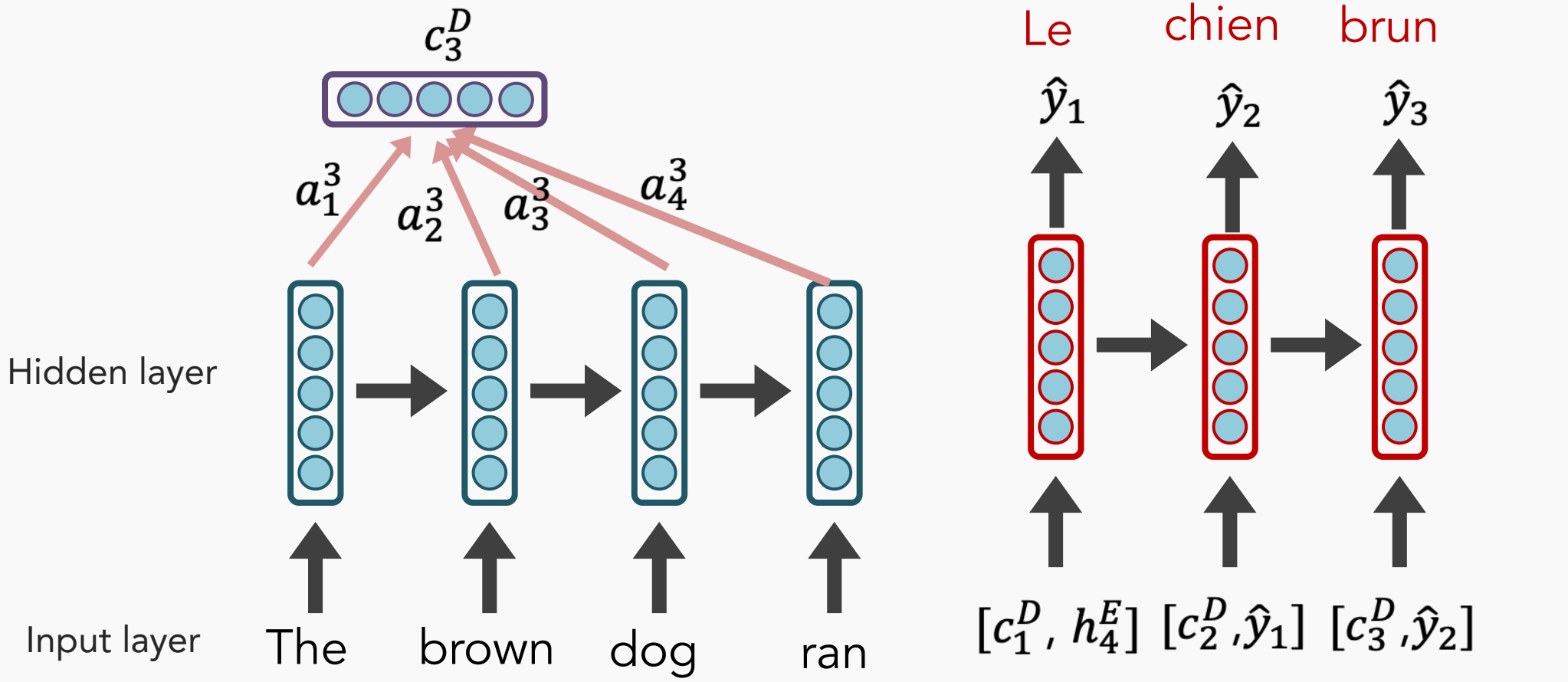

ENCODER RNN

DECODER RNN

seq2seq + Attention

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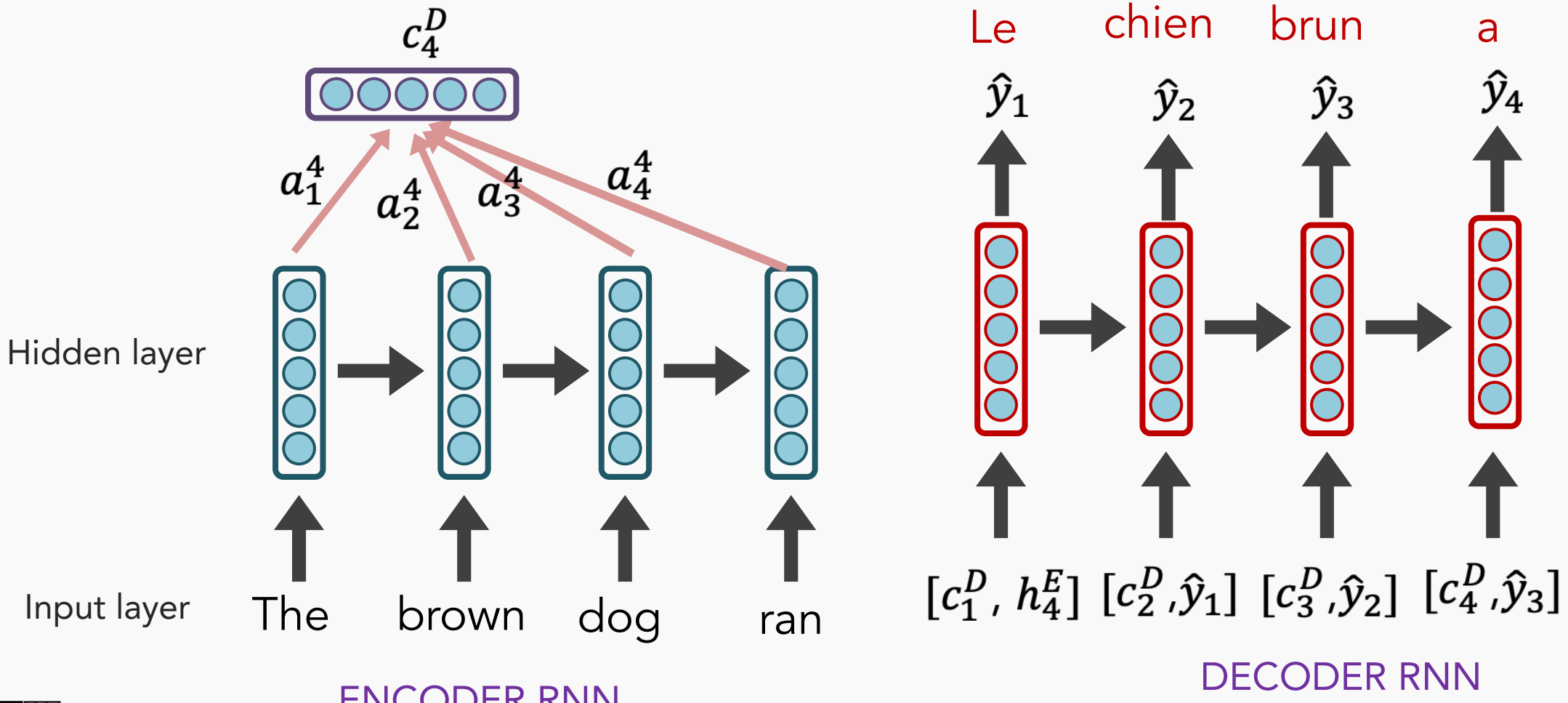

seq2seq + Attention

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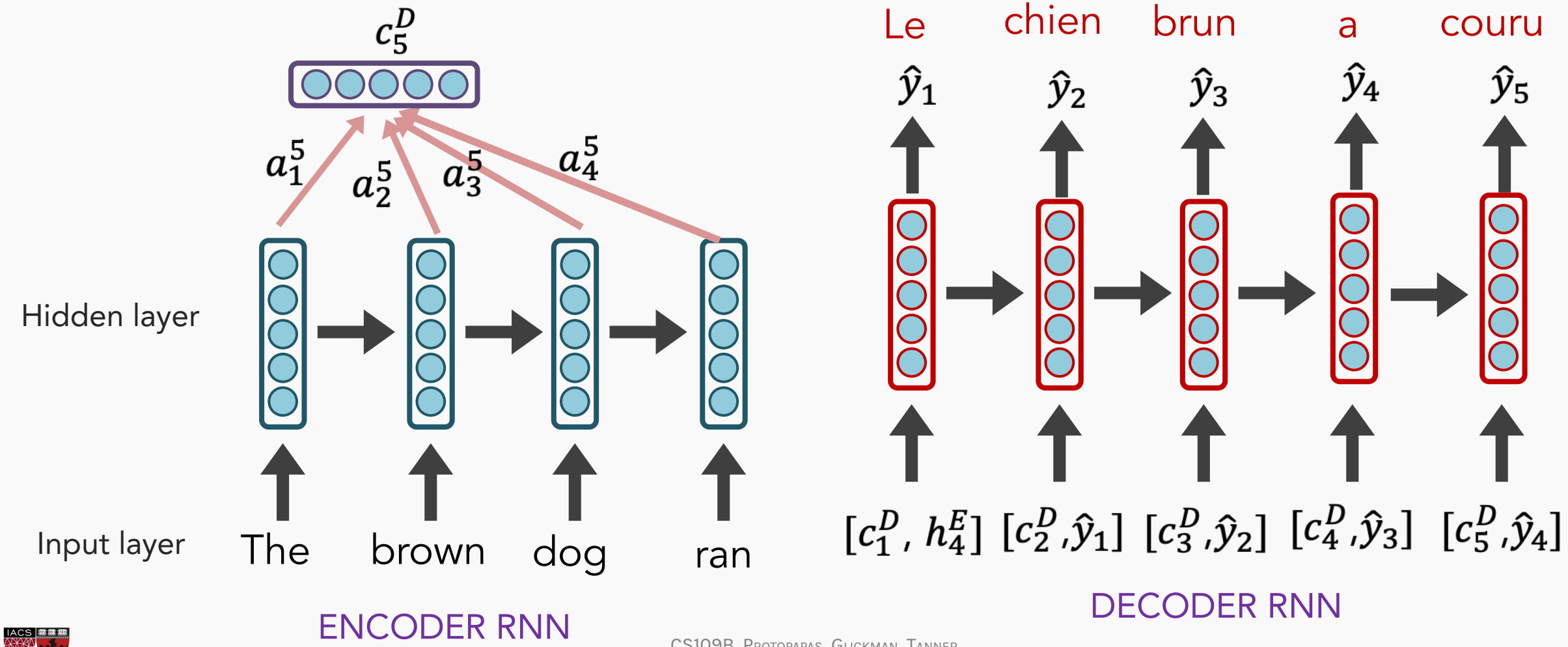


seq2seq + Attention

Attention:

- greatly improves seq2seq results
- allows us to visualize the contribution each word gave during each step of the decoder

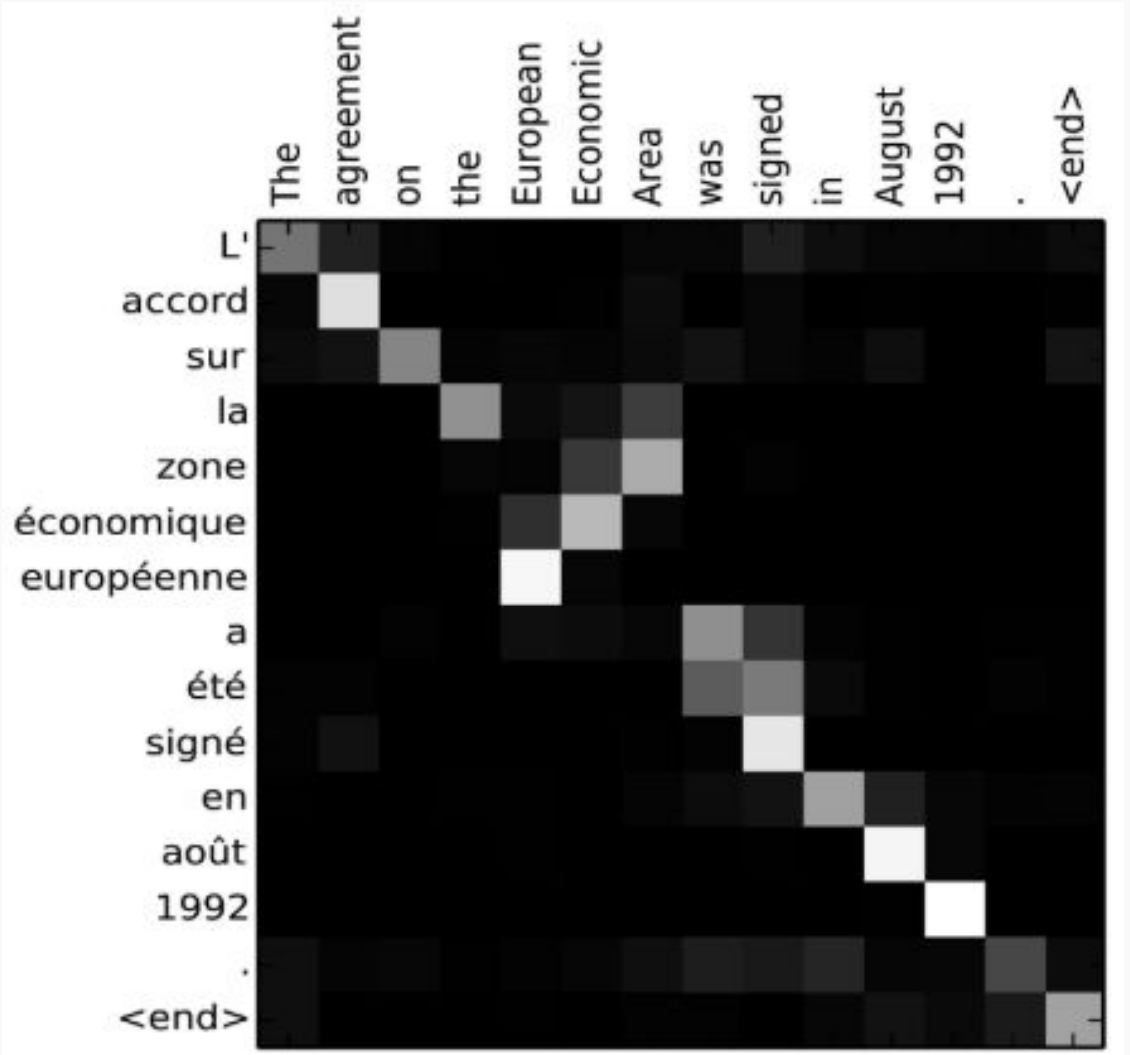
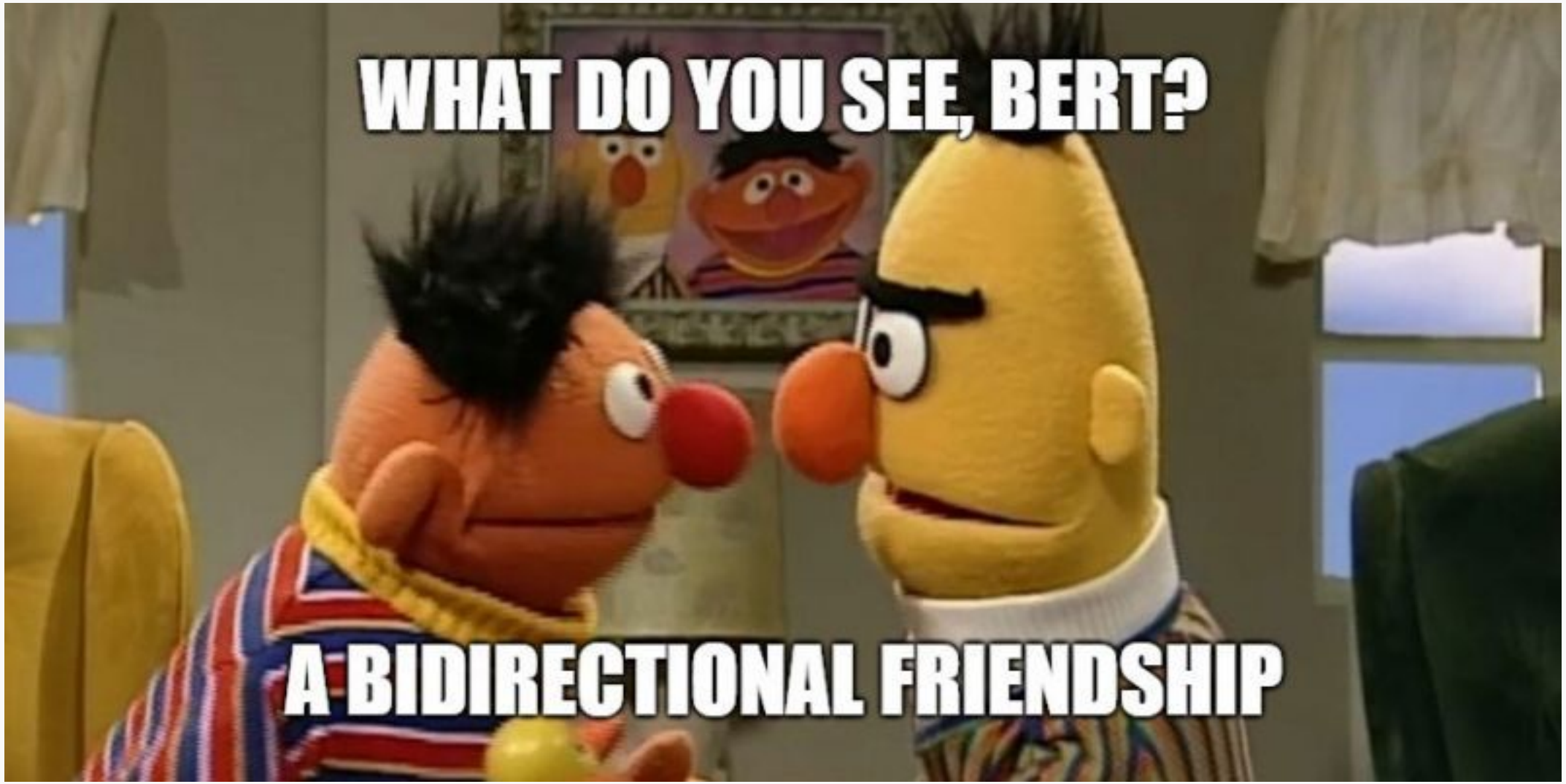


Image source: Fig 3 in Bahdanau et al., 2015

Outline

- Seq2Seq +Attention
- **Transformers +BERT**
- Embeddings


WHAT DO YOU SEE, BERT?
A BIDIRECTIONAL FRIENDSHIP

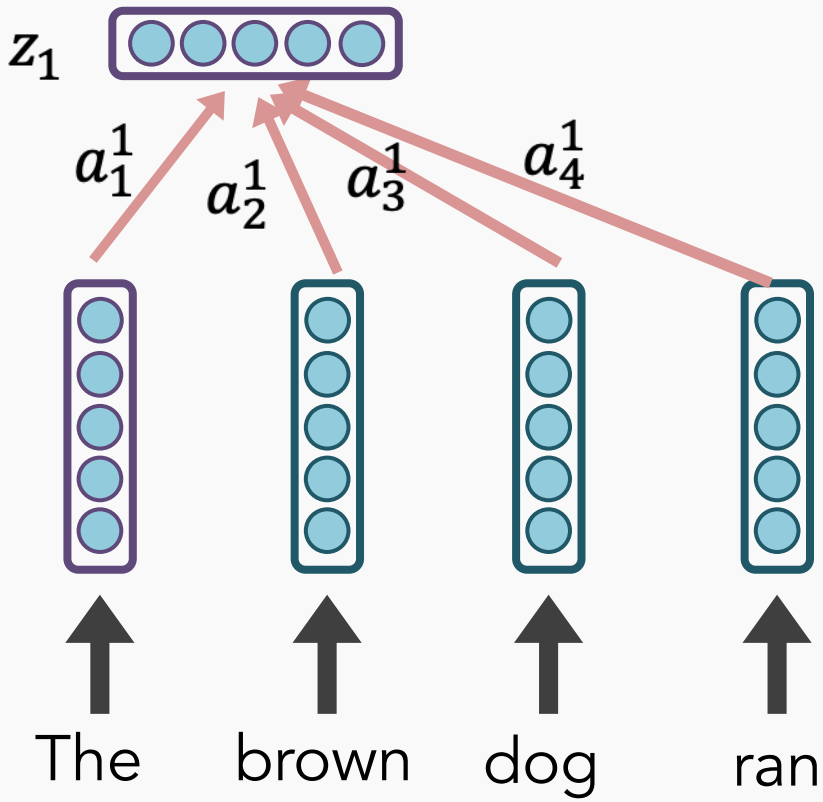
Self-Attention

- Models direct relationships between all words in a given sequence (e.g., sentence)
- Does not concern a seq2seq (i.e., encoder-decoder RNN) framework
- Each word in a sequence can be transformed into an abstract **representation** (embedding) based on the weighted sums of the other words in the same sequence

Self-Attention

Output representation

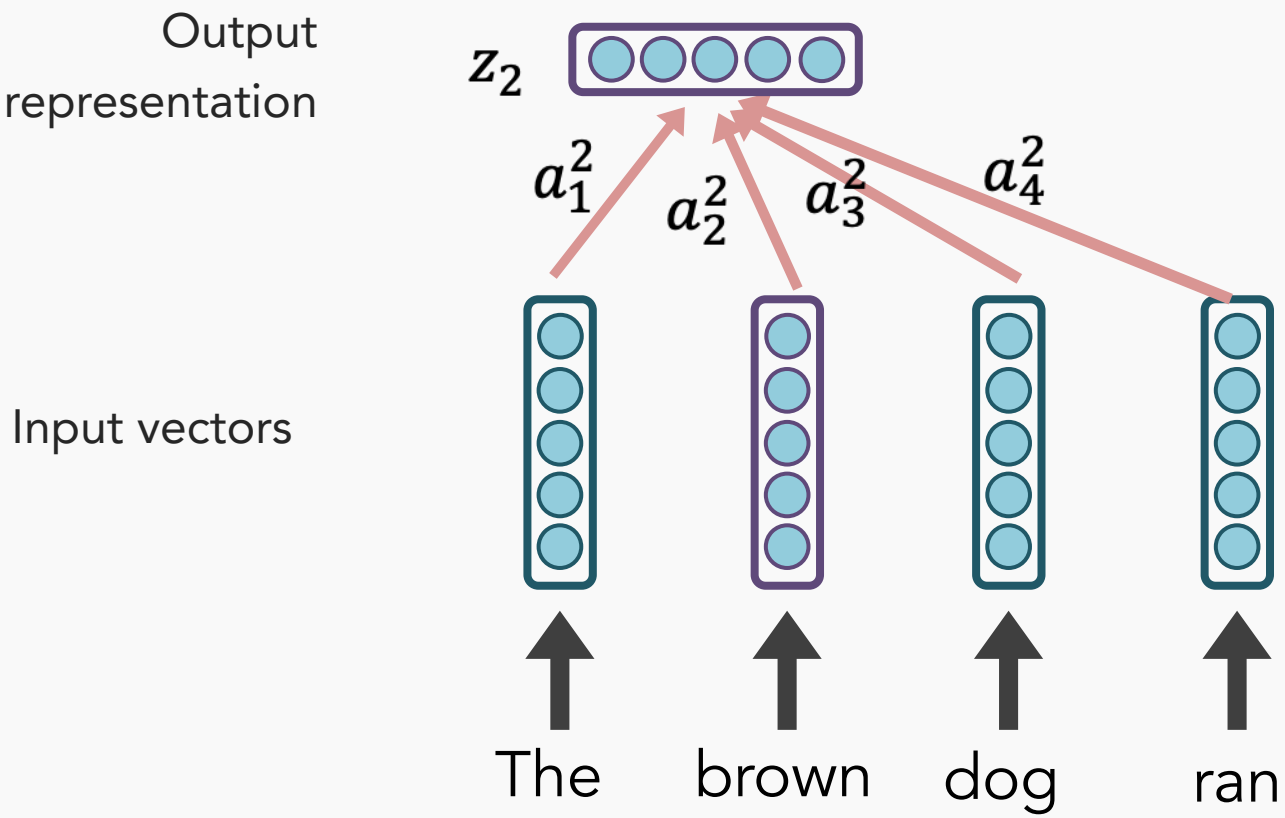
Input vectors



This is a large simplification.

The representations are created from using Query, Key, and Value vectors, produced from learned weight matrices during Training

Self-Attention



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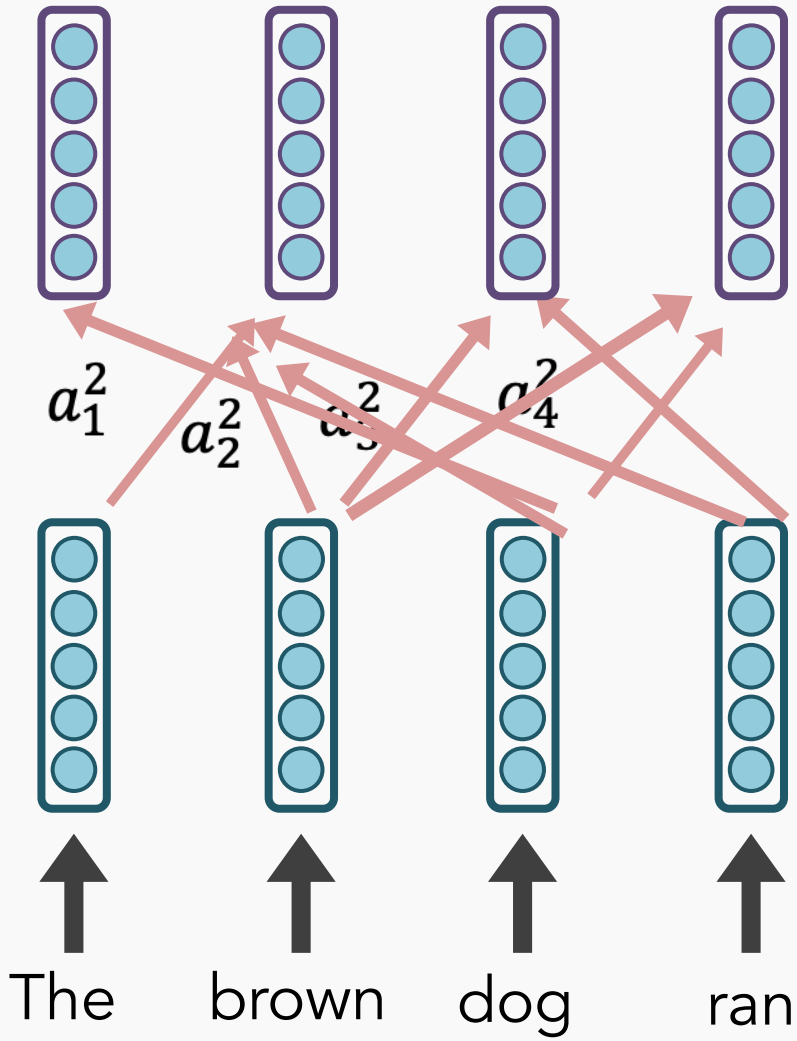

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Self-Attention

To recap:

- Attention determines which pieces of sequence A are most relevant w.r.t. sequence B
- Self-attention determines which pieces of sequence A are most relevant w.r.t. sequence A
- A Transformer combines both; it has an encoder-decoder component, yet also uses self-attention to refine each respective sequence's representation

Self-Attention

- Transformers yield the best results for machine translation (seq2seq)
- Transformers handle long-range dependencies better than LSTMs
- BERT is an example of a Transformer

BERT

- BERT is like the encoder portion of a Transformer
- Uses self-attention
- Uses bi-directional conditioning to perform language modelling
- Yet, it doesn't see its own words because it cleverly masks 15% of its words
- Fine-tunes on a sentence/entailment task
- BERT provides generalized contextual embeddings which can be fine-tuned toward other classification tasks (e.g., sentiment classification)

Conclusion

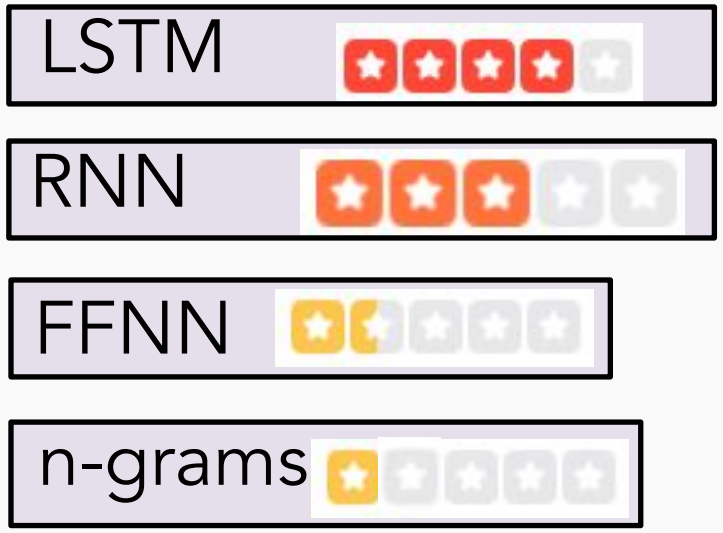
- There has been significant progress in the past few years.
- Some of the complex models are incredible, but rely on having a lot of data and computational resources (e.g., Transformers)
- With all data science and machine learning, it's best to understand your data and your task very well, then clean the data, and start with a simple model (instead of jumping to the most complex model)

Conclusion

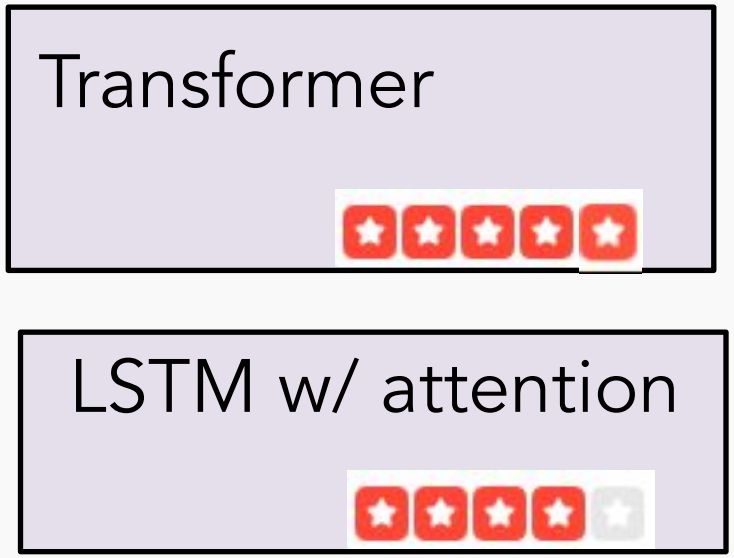
Models

- **N-gram**: count statistics; **elementary** sequence modelling
- **FFNN**: fixed-length context window; basic sequence modelling
- **(Vanilla) RNN**: uses context; fair sequence modelling
- **LSTM**: great contextual usage; great sequence modelling
- **Seq2Seq**: maps 1 sequence to another
- **Attention**: determines which elements in sequence A pertain to sequence B
- **Self-Attention**: determines great representations for items in a sequence
- **Transformers**: learns excellent representation, via a seq2seq framework and self-attention

Sequential Modelling



Sequence Modelling
(1-to-1 mapping)



seq2seq

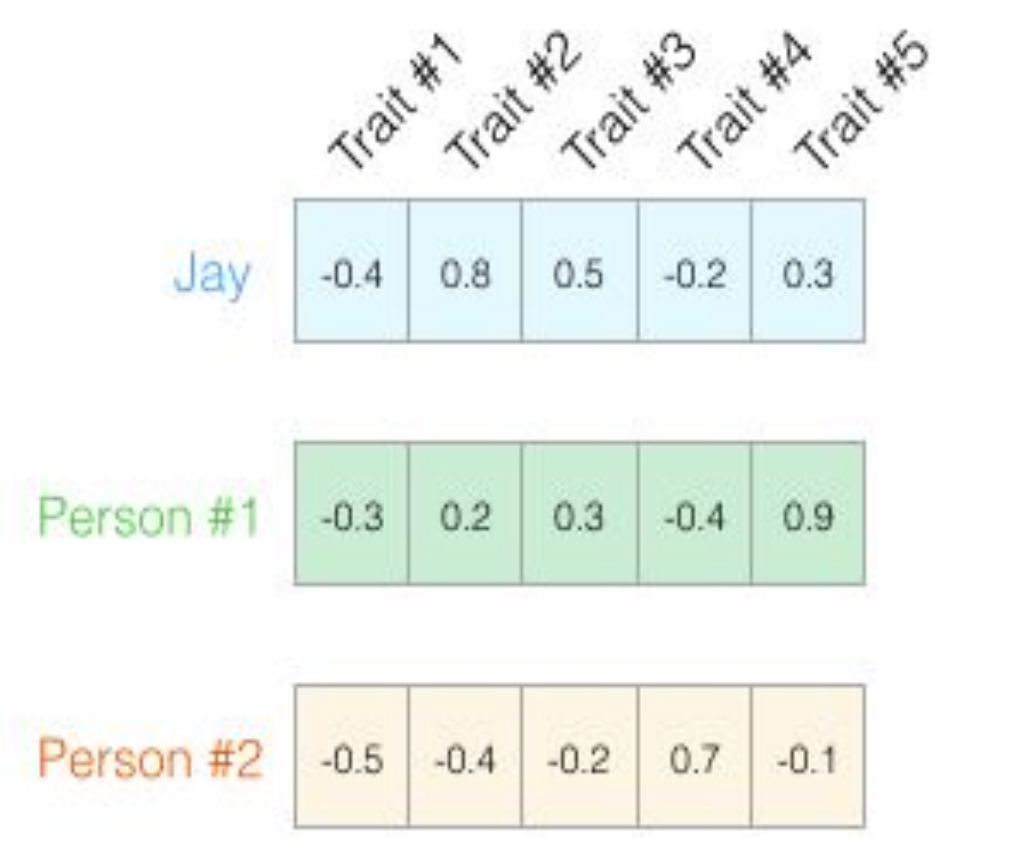
Credit & further resources:

- Backprop: http://cs231n.github.io/optimization-2/
- Abigail See's lectures: http://web.stanford.edu/class/cs224n/index.html
- Illustrated BERT: http://jalammar.github.io/illustrated-bert/
- Andrew Ng (Attention): https://www.youtube.com/watch?v=quoGRI-1l0A
- Illustrated Transformer: https://jalammar.github.io/illustrated-transformer/
- Google (Transformers): https://ai.googleblog.com/2017/08/transformer-novel-neural-network.html
- ELMo paper: https://arxiv.org/pdf/1802.05365.pdf

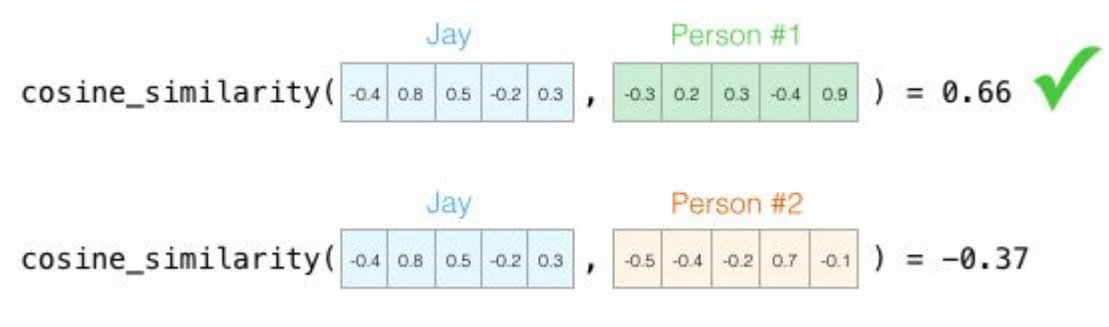
Outline

- Seq2Seq +Attention
- Transformers +BERT
- **Embeddings**

The basics idea



- Observe a bunch of people
- **Infer** personality traits from them
- Vector of traits is called an **Embedding**
- Who is more similar? Jay and who?
- Use Cosine Similarity of the vectors



Images by Jay Alammar

Categorical Data

Example:

Rossmann Kaggle Competition: Rossmann is a 3000 store European Drug Store Chain. The idea is to predict sales 6 weeks in advance.

Consider `store_id` as an example. This is a **categorical** predictor, i.e. values come from a finite set.

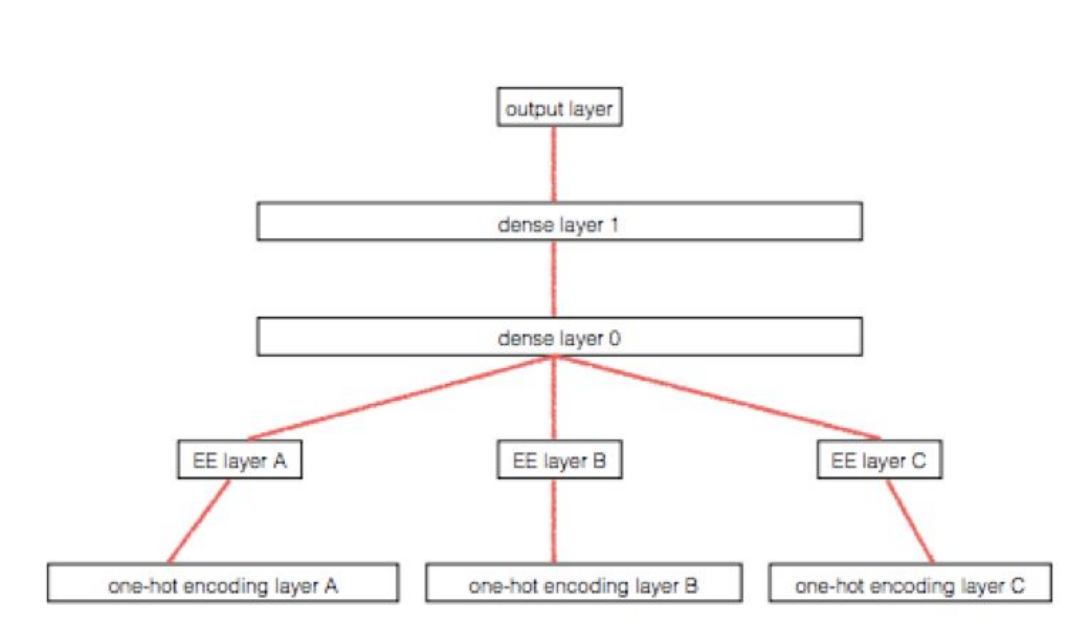
We usually **one-hot encode** this: a single store is a length 3000 bit-vector with one bit flipped on.

Categorical Data

What is the problem with this?

- The 3000 stores have commonalities, but the one-hot encoding does not represent this.
- Indeed the dot-product (cosine similarity) of any two 1-hot bitmaps must be 0.
- Would be useful to learn a lower-dimensional **embedding** for the purpose of sales prediction.
- These store "personalities" could then be used in other models (different from the model used to learn the embedding) for sales prediction.
- The embedding can be also used for other **tasks**, such as employee turnover prediction.

Training an Embedding



- Normally you would do a linear or MLP regression with sales as the target, and both continuous and categorical features.
- The game is to replace the 1-hot encoded categorical features by "lower-width" embedding features, for *each* categorical predictor.
- This is equivalent to considering a neural network with the output of an additional **Embedding Layer** concatenated in.
- The Embedding layer is simply a linear regression.

Image from Guo and Berkhahn

Training an Embedding (cont)

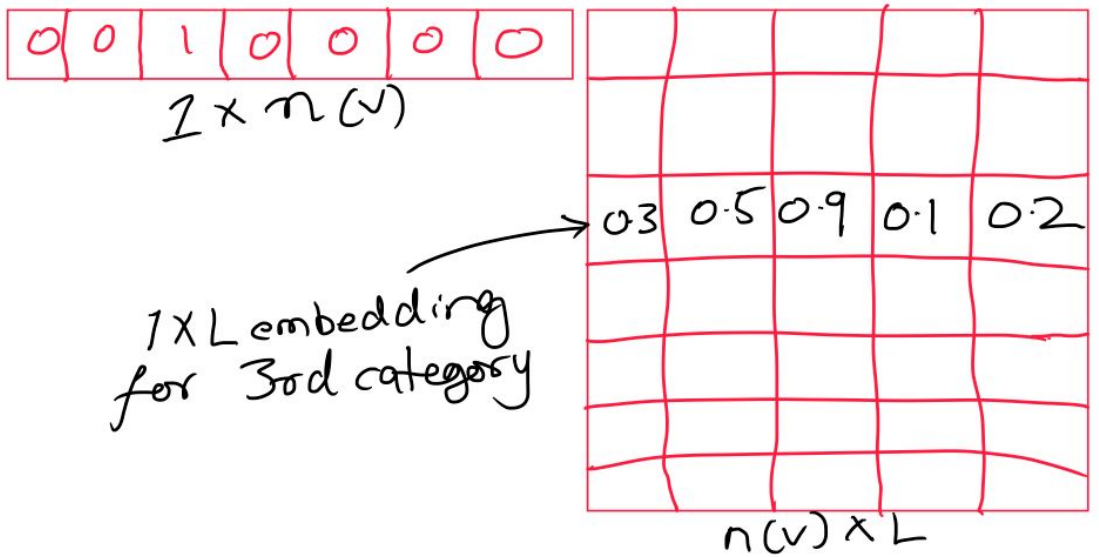
A 1-hot vector for a categorical variable with cardinality can be written using the Kronecker Delta symbol as:

$$v_k = \delta_{jk}, j \in \{1, \ldots, N(v)\}$$

Then an embedding of width (dimension) L is just a $N(v) \times L$ matrix of weights W_{ij} such that multiplying the k^{th} 1-hot vector by this weight matrix picks out the k^{th} row of weights (see right).

But how do we find these weights?

We fit for them with the rest of the weights in the MLP!



Training an Embedding (cont)

```
def build_keras_model():
    input_cat = []
    output_embeddings = []
    for k in cat_vars+nacols_cat: #categoricals plus NA booleans
        input_1d = Input(shape=(1,))
        output_1d = Embedding(input_cardinality[k], embedding_cardinality[k], name='{}_embedding'.format(k))(input_1d)
        output = Reshape(target_shape=(embedding_cardinality[k],))(output_1d)
        input_cat.append(input_1d)
        output_embeddings.append(output)

    main_input = Input(shape=(len(cont_vars),), name='main_input')
    output_model = Concatenate()([main_input, *output_embeddings])
    output_model = Dense(1000, kernel_initializer="uniform")(output_model)
    output_model = Activation('relu')(output_model)
    output_model = Dense(500, kernel_initializer="uniform")(output_model)
    output_model = Activation('relu')(output_model)
    output_model = Dense(1)(output_model)

    kmodel = KerasModel(
        inputs=[*input_cat, main_input],
        outputs=output_model
    )
    kmodel.compile(loss='mean_squared_error', optimizer='adam')
    return kmodel

def fitmodel(kmodel, Xtr, ytr, Xval, yval, epochs, bs):
    h = kmodel.fit(Xtr, ytr, validation_data=(Xval, yval),
                       epochs=epochs, batch_size=bs)
    return h
```

Embedding is just a linear regression

So why are we giving it another name?

- it is usually to lower the dimensional space
- traditionally we have done linear dimensional reduction through PCA and truncation, but sparsity can throw a spanner into the works.
- we train the weights of the embedding regression using gradient descent (or stochastic gradient descent), along with the weights of the downstream task (here prediting the sales 6 weeks in advanced).
- the embedding can be used for alternate tasks, such as finding the similarity of users.

See how Spotify does all this.

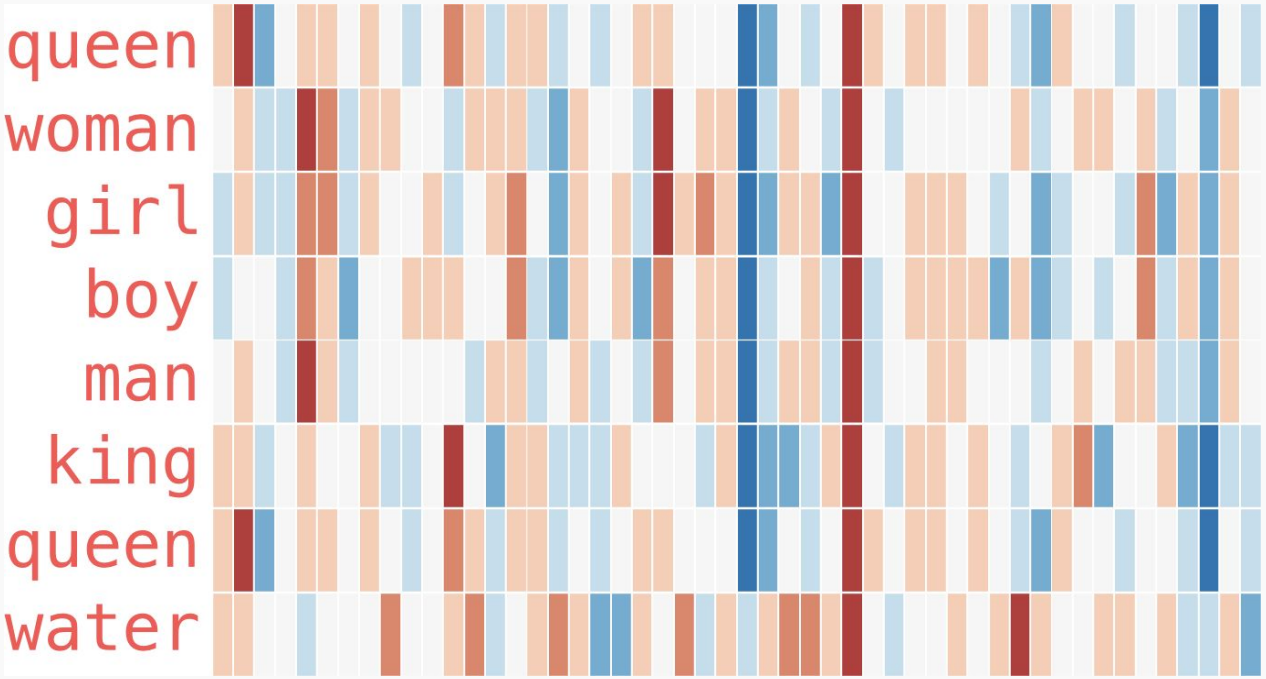
```
def embedding_input(emb_name, n_items, n_fact=20, l2regularizer=1e-4):
    inp = Input(shape=(1,), dtype='int64', name=emb_name)
    return inp, Embedding(n_items, n_fact, input_length=1, embeddings_regularizer=l2(l2regularizer))(inp)

usr_inp, usr_emb = embedding_input('user_in', n_users, n_fact=50, l2regularizer=1e-4)
mov_inp, mov_emb = embedding_input('movie_in', n_movies, n_fact=50, l2regularizer=1e-4)

def create_bias(inp, n_items):
    x = Embedding(n_items, 1, input_length=1)(inp)
    return Flatten()(x)

usr_bias = create_bias(usr_inp, n_users)
mov_bias = create_bias(mov_inp, n_movies)

def build_dp_bias_recommender(u_in, m_in, u_emb, m_emb, u_bias, m_bias):
    x = dot([u_emb, m_emb], axes=(2,2))
    x = Flatten()(x)
    x = add([x, u_bias])
    x = add([x, m_bias])
    bias_model = Model([u_in, m_in], x)
    bias_model.compile(Adam(0.001), loss='mse')
    return bias_model

bias_model = build_dp_bias_recommender(usr_inp, mov_inp, usr_emb, mov_emb, usr_bias, mov_bias)
```

Word Embeddings

- the vocabulary V of a corpus (large swath of text) can have 10,000 and maybe more words.
- a 1-hot encoding is huge, moreover, similarities between words cannot be established.
- we map words to a smaller dimensional latent space of size L by considering some downstream task to train on.
- we hope that the embeddings learned are useful for other tasks.

images in this section from Illustrated word2vec

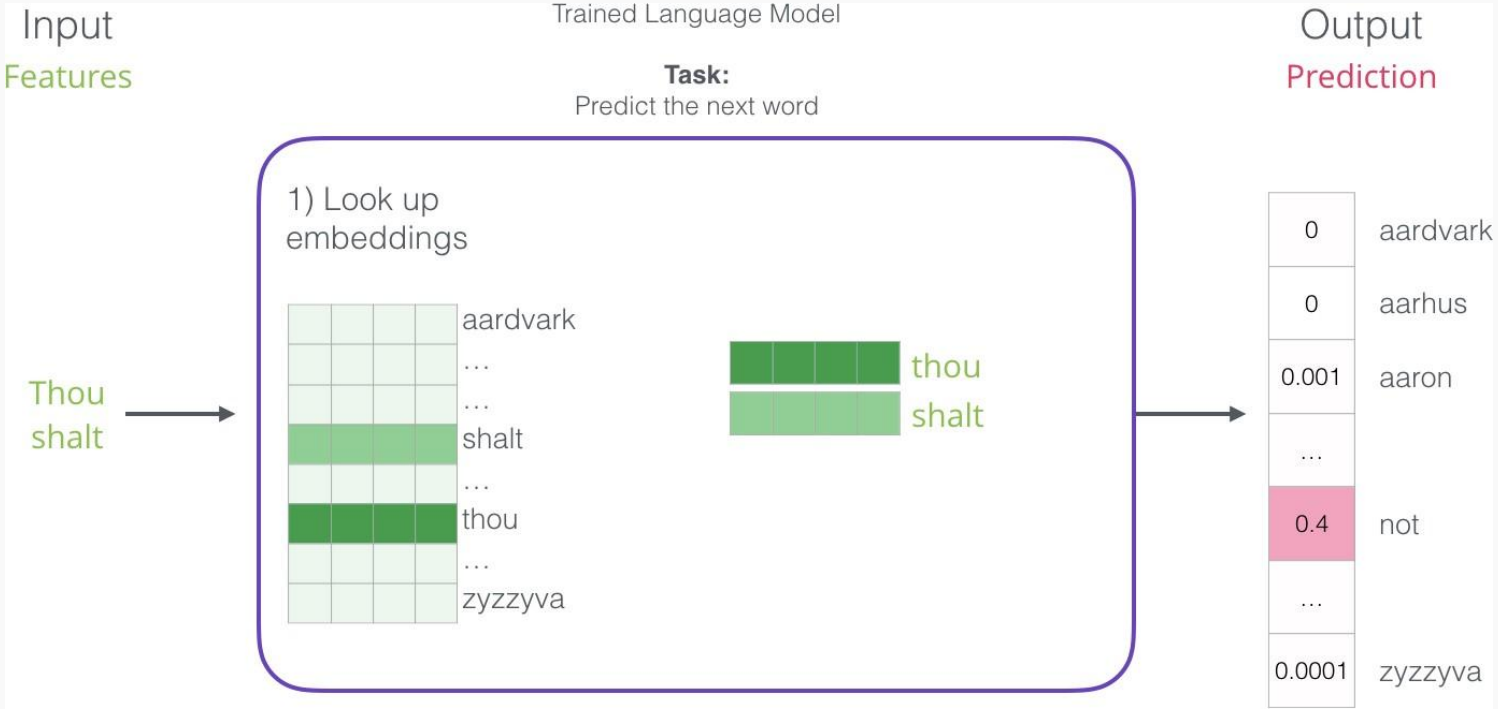
Obligatory example



See man->boy as woman->girl, similarities of king and queen, for e.g. These are lower dimensional GloVe embedding vector.

How do we train word embeddings?

- We need to choose a downstream task.
- We could choose **Language Modeling**: predict the next word.
- We'll start with random "weights" for the embeddings and other parameters and start learning.
- A trained model+embeddings would look like this:



How do we set up a training set?

Thou shalt not make a machine in the likeness of a human mind

Sliding window across running text

thou	shalt	not	make	a	machine	in	the	…
thou	shalt	not	make	a	machine	in	the	
thou	shalt	not	make	a	machine	in	the	
thou	shalt	not	make	a	machine	in	the	
thou	shalt	not	make	a	machine	in	the	

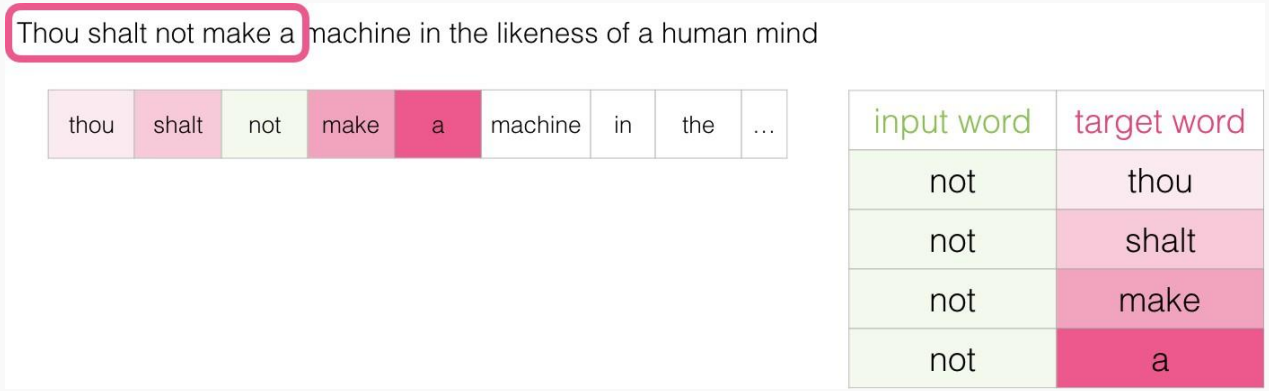
Dataset

input 1	input 2	output
thou	shalt	not
shalt	not	make
not	make	a
make	a	machine
a	machine	in

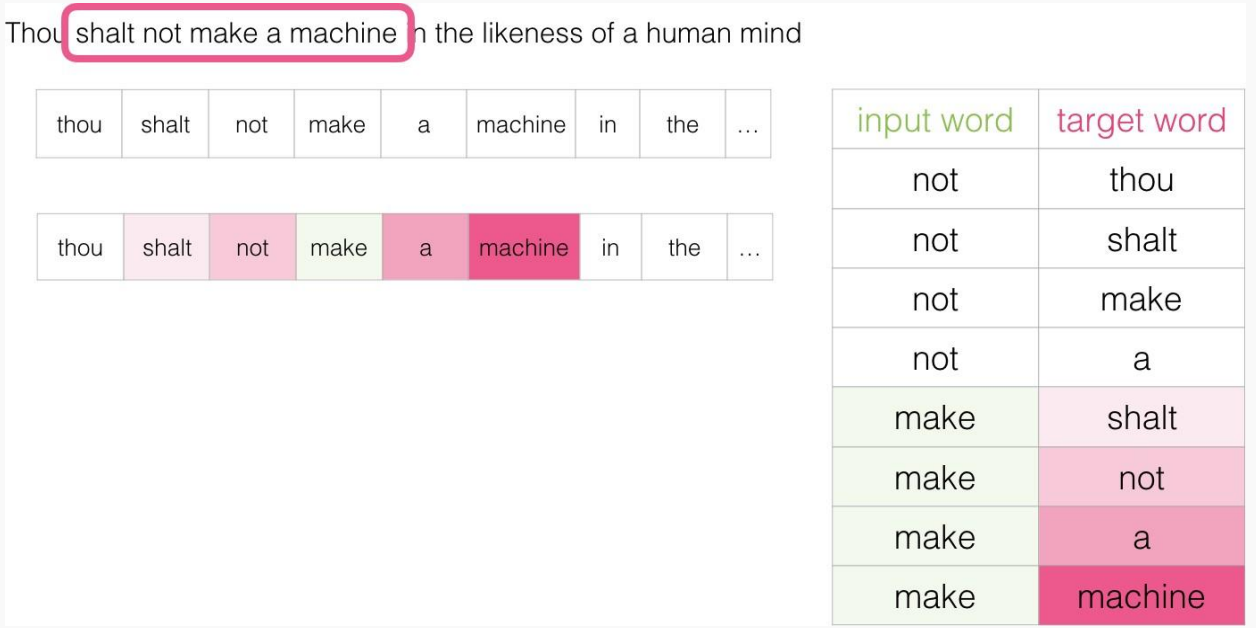
Why not look both ways? This leads to the Skip-Gram and CBOW architectures..

SKIP-GRAM: Predict Surrounding Words

Choose a window size (here 4) and construct a dataset by sliding a window across.



input word	target word
not	thou
not	shalt
not	make
not	a

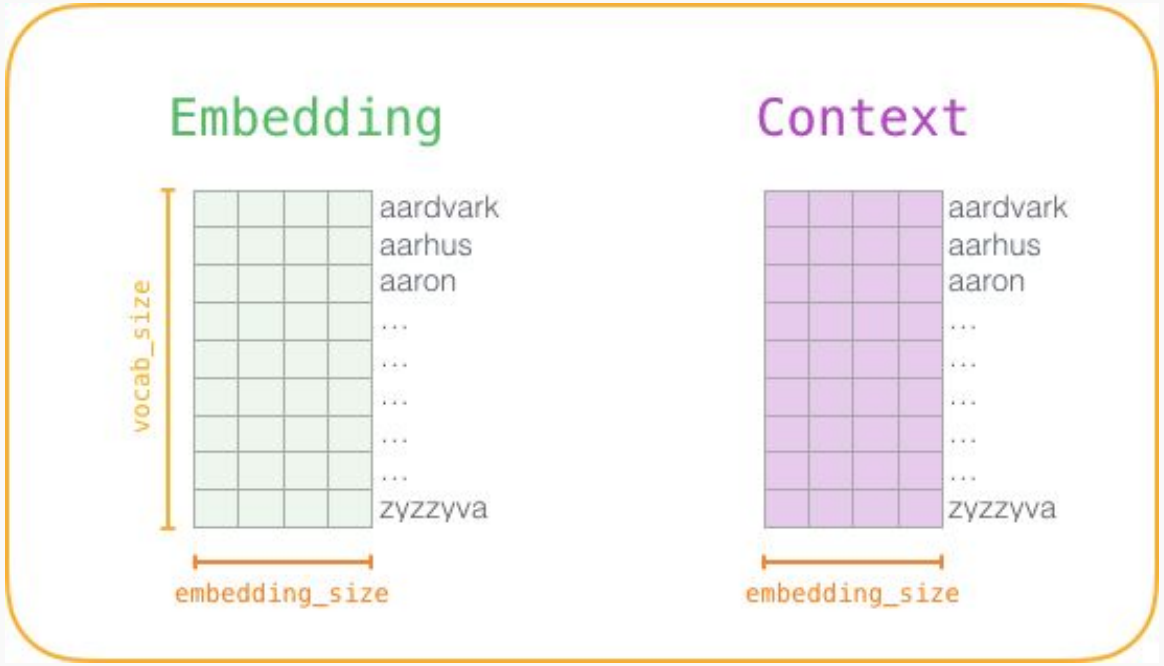


input word	target word
not	thou
not	shalt
not	make
not	a
make	shalt
make	not
make	a
make	machine

SKIP-GRAM: Details

We assume that, Naive Bayes style, the joint probability of all **context** words in a window conditioned on the central word (w_c) is the product of the individual conditional probabilities:

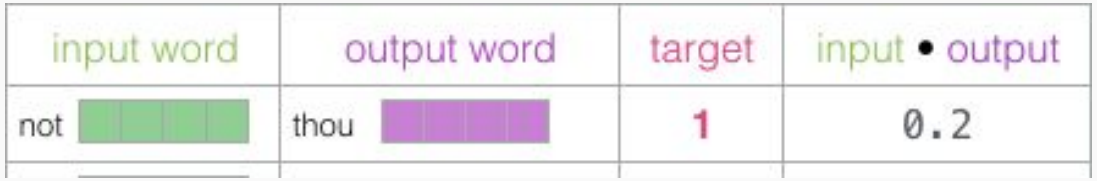
$$P(\{w_o\} \mid w_c) = \prod_{i \in window} p(w_{oi} \mid w_c)$$



Now assume that each word is represented as 2 embeddings, an **input** embedding (v_c) when we talk about the central word and a context embedding (u_o) when we talk about the surrounding window.

The probability of an output word, given a central word, is assumed to be given by a softmax of the dot product of the embeddings.

$$\mathbb{P}(w_o \mid w_c) = \frac{\exp(\boldsymbol{u}_o^\top \boldsymbol{v}_c)}{\sum_{i \in \mathcal{V}} \exp(\boldsymbol{u}_i^\top \boldsymbol{v}_c)},$$

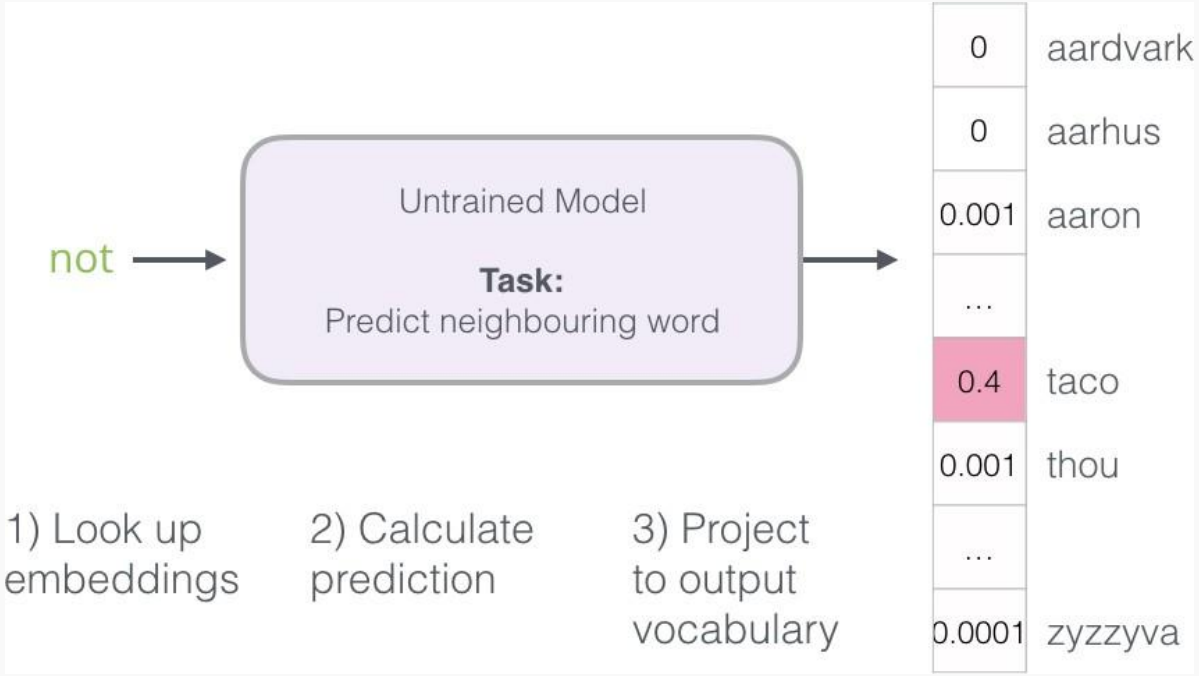


Then, assuming a text sequence of length T and window size m, the likelihood function is:

$$\mathcal{L} = \prod_{t=1}^{T} \prod_{-m \leq j \leq m,\ j \neq 0} \mathbb{P}(w^{(t+j)} \mid w^{(t)}).$$

We'll use the Negative Log Likelihood as loss (NLL)

Prediction



With random initial weights , we make a prediction for surrounding words, and calculate the NLL for the prediction. We then backpropagate the NLL's gradients to find new weights and repeat

Consider two sentences: "*I am running.*" and "*I am writing.*". "I" and "am" targets will backprop to same **input** embedding and so, after some training, "writing" and "running" will be highly correlated. Appropriate correlations will emerge as corpus size increases.

Problems

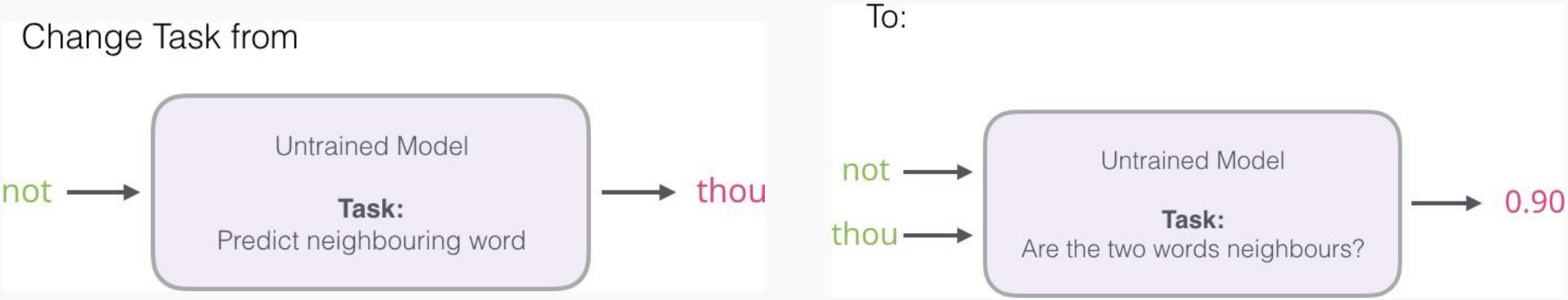
$$\mathbb{P}(w_o \mid w_c) = \frac{\exp(\boldsymbol{u}_o^\top \boldsymbol{v}_c)}{\sum_{i \in \mathcal{V}} \exp(\boldsymbol{u}_i^\top \boldsymbol{v}_c)},$$

- in the forward mode, the calculation of softmax requires a sum over the entire vocabulary
- in the backward mode, the gradients need this sum too. For example:

$$\frac{\partial \log P(w_o \mid w_c)}{\partial \boldsymbol{v}_c} = \boldsymbol{u}_o - \sum_{j \in \mathcal{V}} P(w_j \mid w_c) \boldsymbol{u}_j.$$

For large vocabularies, this is very expensive!

Changing Tasks



Changing from predicting neighbors to "*are we neighbors?*" changes model from neural net to logistic regression.

Changing Tasks (cont)

We'll now thus choose $P(D=1|w_c, w_o) = \sigma(u_o^T v_c)$ and will maximize the likelihood:

$$\mathcal{L} = \prod_{t=1}^{T} \prod_{-m \le j \le m,\ j \ne 0} P(D=1 \mid w^{(t)}, w^{(t+j)}).$$

But the response variable in the dataset changes to all 1's and a trivial classifier always returning 1 will give the best score. Not good (this is equivalent to all embeddings being equal and infinite)!

Negative Sampling

input word	target word
not	thou
not	shalt
not	make
not	a
make	shalt
make	not
make	a
make	machine

input word	output word	target
not	thou	1
not	shalt	1
not	make	1
not	a	1
make	shalt	1
make	not	1
make	a	1
make	machine	1

To fix we randomly choose words from our vocabulary and label them with 0.

Pick randomly from vocabulary (random sampling)

input word	output word	target
not	thou	1
not	aaron	0
not	taco	0
not	shalt	1
not	make	1

Likelihood model

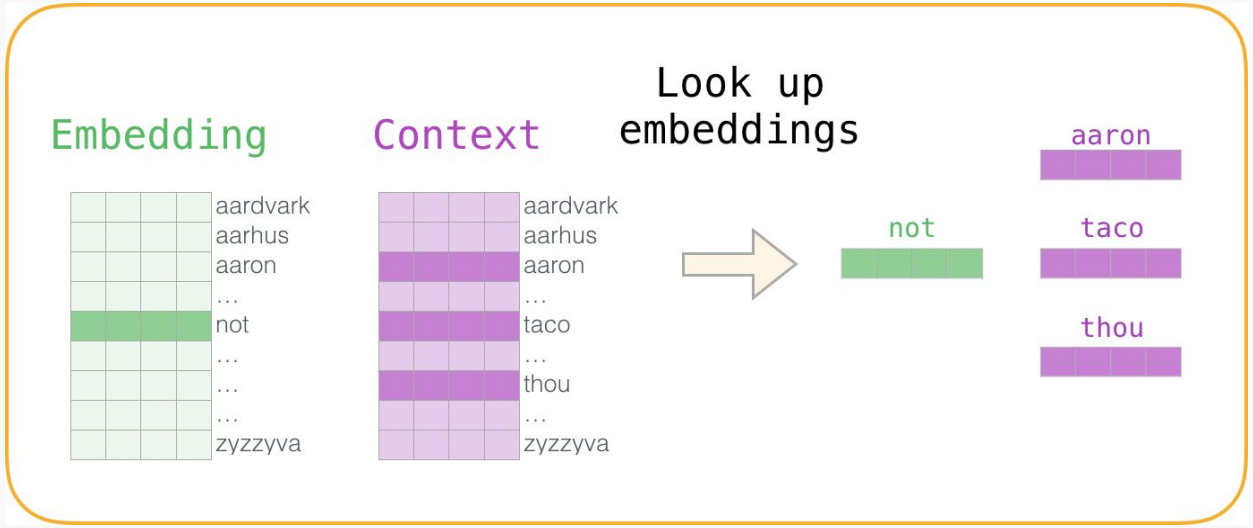
We go back to the old likelihood: $$\mathcal{L} = \prod_{t=1}^{T} \prod_{-m \leq j \leq m,\ j \neq 0} \mathbb{P}(w^{(t+j)} \mid w^{(t)}).$$

But now, the probability is approximated using negative sampling as:

$$P(w^{(t+j)} \mid w^{(t)}) = P(D = 1 \mid w^{(t)}, w^{(t+j)}) \prod_{k=1,\ w_k \sim P(w)}^{K} P(D = 0 \mid w^{(t)}, w_k).$$

The NLL now has a sum over a K--sized window, rather than the full vocabulary.

Training the model



- The negative sampling probabilities are now sigmoids subtracted from 1, whereas the positives are simply sigmoids.
- We now compute the loss, and repeat over training examples in our batch.
- And backpropagate to obtain gradients and change the embeddings and weights some, for each batch, in each epoch

input word	output word	target	input • output	sigmoid()
not	thou	1	0.2	0.55
not	aaron	0	-1.11	0.25
not	taco	0	0.74	0.68

```
def make_model(vector_dim, vocab_size, learn_rate):
    stddev = 1.0 / vector_dim
    initializer = RandomNormal(mean=0.0, stddev=stddev, seed=None)

    word_input = Input(shape=(1,), name="word_input")
    word = Embedding(input_dim=vocab_size, output_dim=vector_dim, input_length=1,
                     name="word_embedding", embeddings_initializer=initializer)(word_input)

    context_input = Input(shape=(1,), name="context_input")
    context = Embedding(input_dim=vocab_size, output_dim=vector_dim, input_length=1,
                     name="context_embedding", embeddings_initializer=initializer)(context_input)

    merged = dot([word, context], axes=2, normalize=False, name="dot")
    merged = Flatten()(merged)
    output = Dense(1, activation='sigmoid', name="output")(merged)

    optimizer = TFOptimizer(tf.train.AdagradOptimizer(learn_rate))
    model = Model(inputs=[word_input, context_input], outputs=output)
    model.compile(loss="binary_crossentropy", optimizer=optimizer)
        self.model = model
```

```
def train(model, sequence, window_size, negative_samples, batch_size):
        """ Trains the word2vec model """

        # in order to balance out more negative samples than positive
        negative_weight = 1.0 / negative_samples
        class_weight = {1: 1.0, 0: negative_weight}
        sequence_length = len(sequence)
        approx_steps_per_epoch = (sequence_length * (
                window_size * 2.0) + sequence_length * negative_samples) / batch_size
        batch_iterator = skip_gram.batch_iterator(sequence, window_size, negative_samples, batch_size)

        model.fit_generator(batch_iterator,
                            steps_per_epoch=approx_steps_per_epoch,
                            epochs=epochs,
                            verbose=verbose,
                            class_weight=class_weight,
                            max_queue_size=100)
```

The result

- We discard the Context matrix, and **save the embeddings matrix**.
- We can use the embeddings matrix for our next task (perhaps a sentiment classifier).
- We could have trained embeddings along with that particular task to make the embeddings sentiment specific. There is always a tension between domain/task specific embeddings and generic ones.
- This tension is usually resolved in favor of using generic embeddings since task specific datasets seem to be smaller
- We can still unfreeze pre-trained embedding layers to modify them for domain specific tasks via transfer learning.

Usage of word2vec

- the pre-trained word2vec and other embeddings (such as GloVe) are used everywhere in NLP today.
- the ideas have been used elsewhere as well. AirBnB and Anghami model sequences of listings and songs using word2vec like techniques.
- Alibaba and Facebook use word2vec and graph embeddings for recommendations and social network analysis.