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

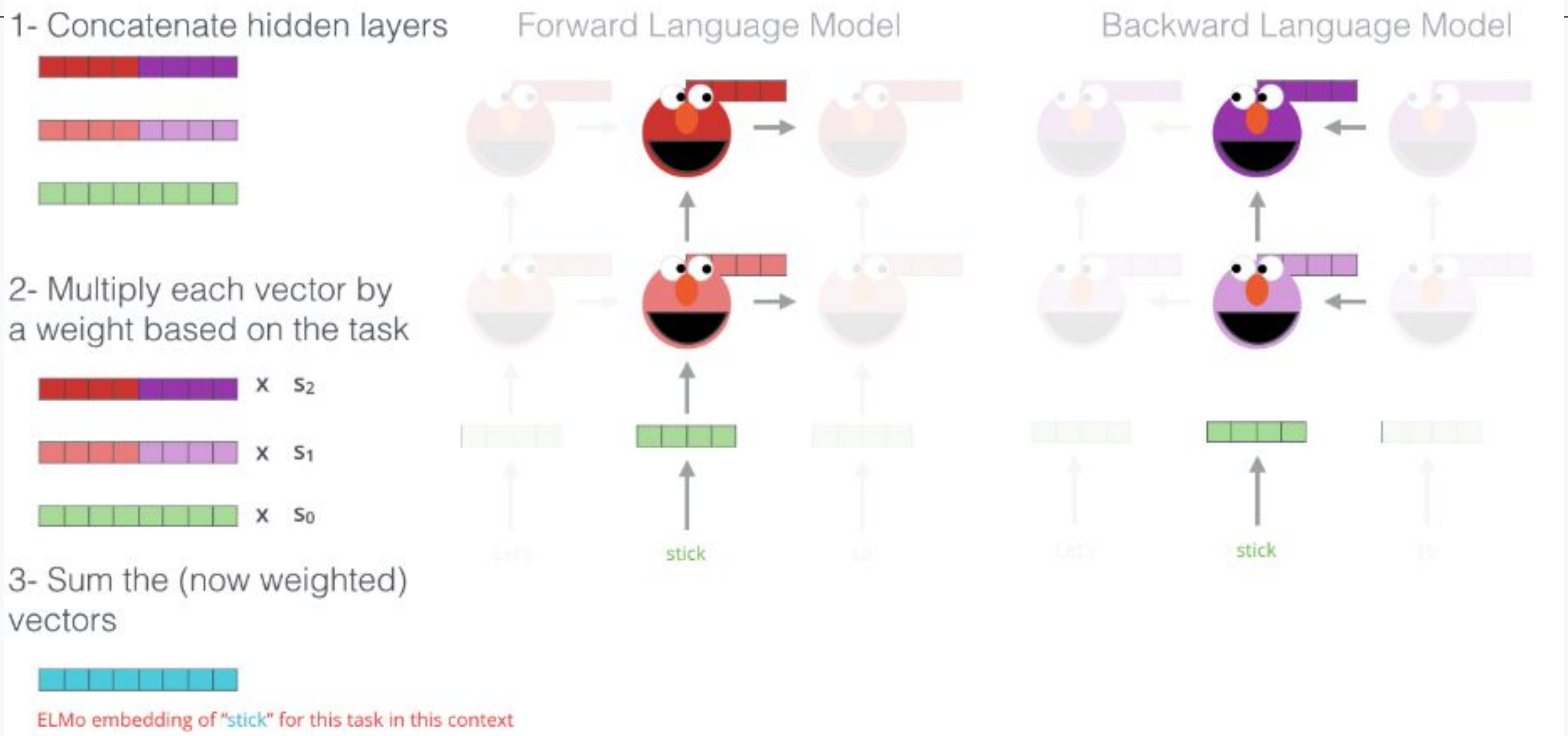


Illustration: http://jalammar.github.io/illustrated-bert/

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

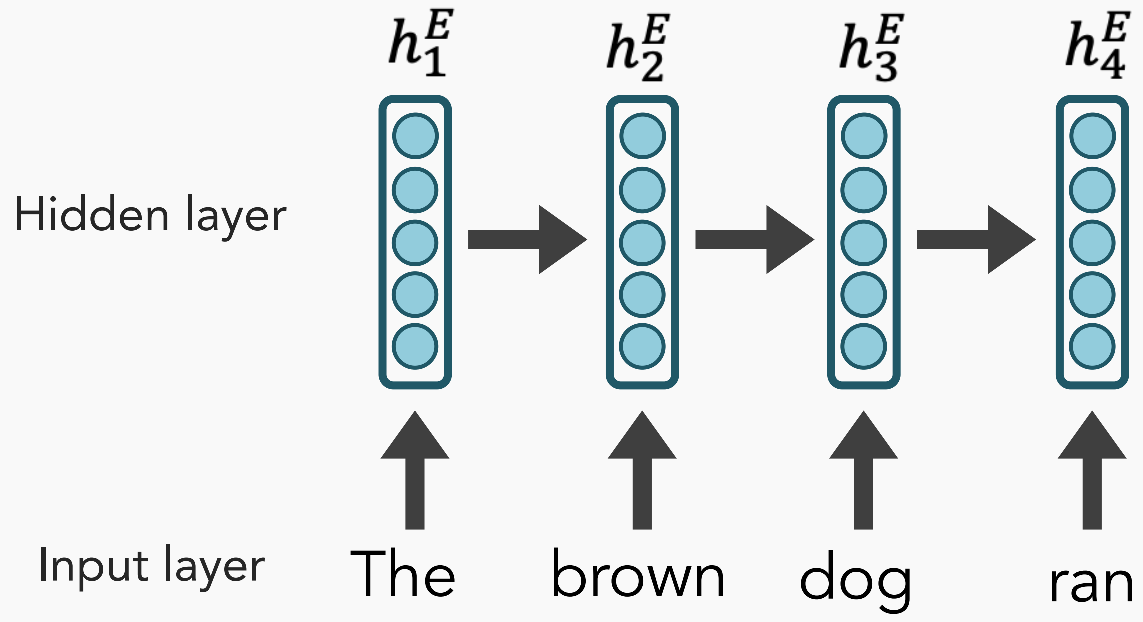
Sequence-to-Sequence (seq2seq)

- 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

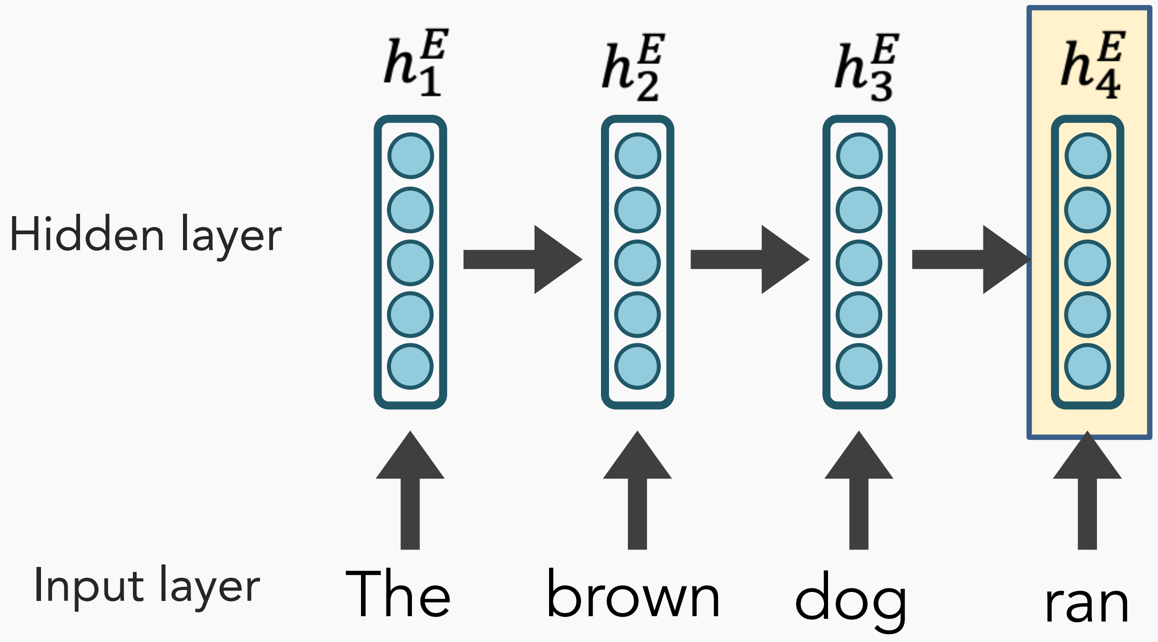
Sequence-to-Sequence (seq2seq)



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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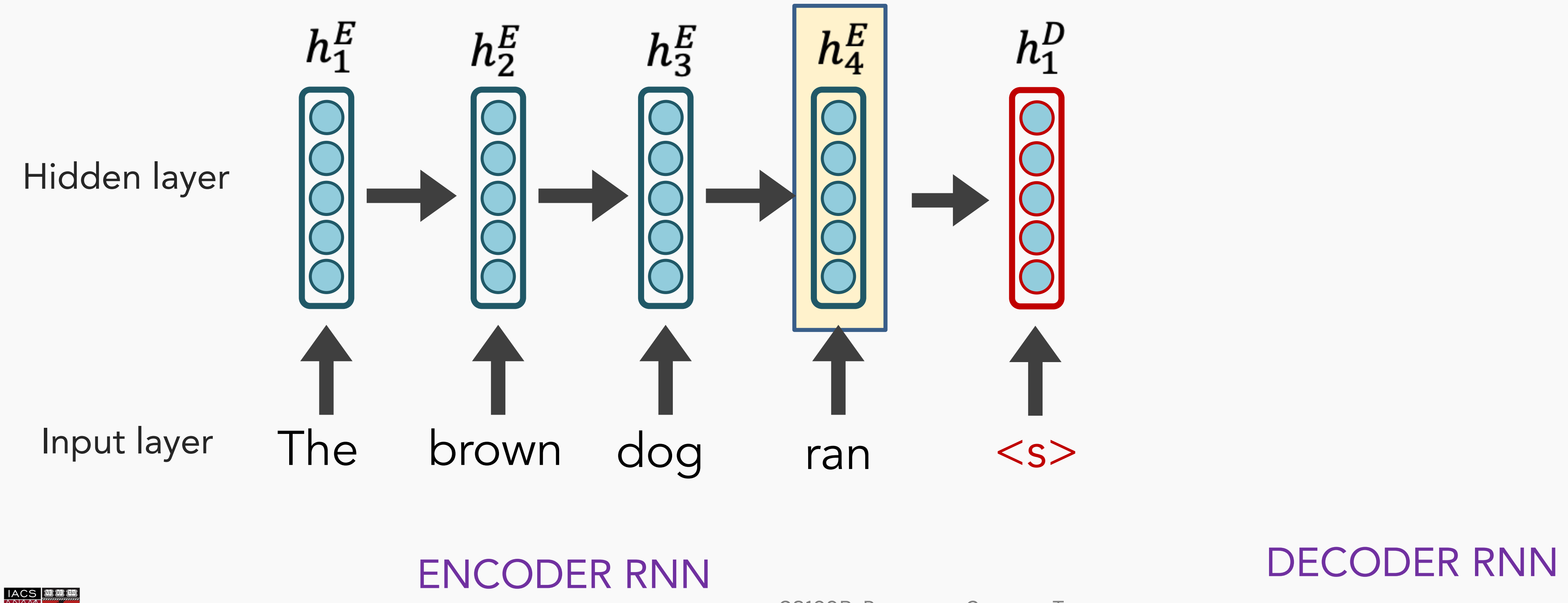

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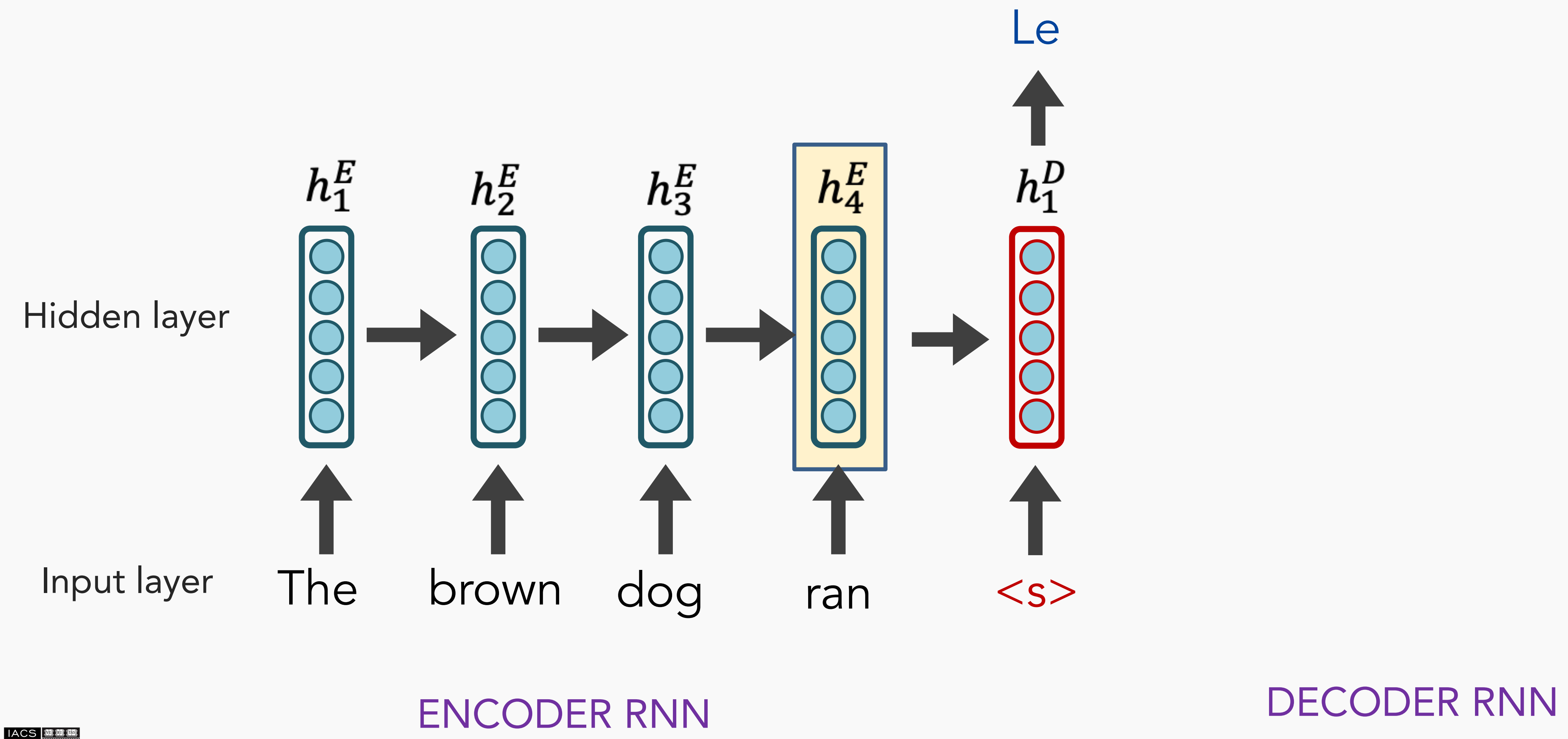

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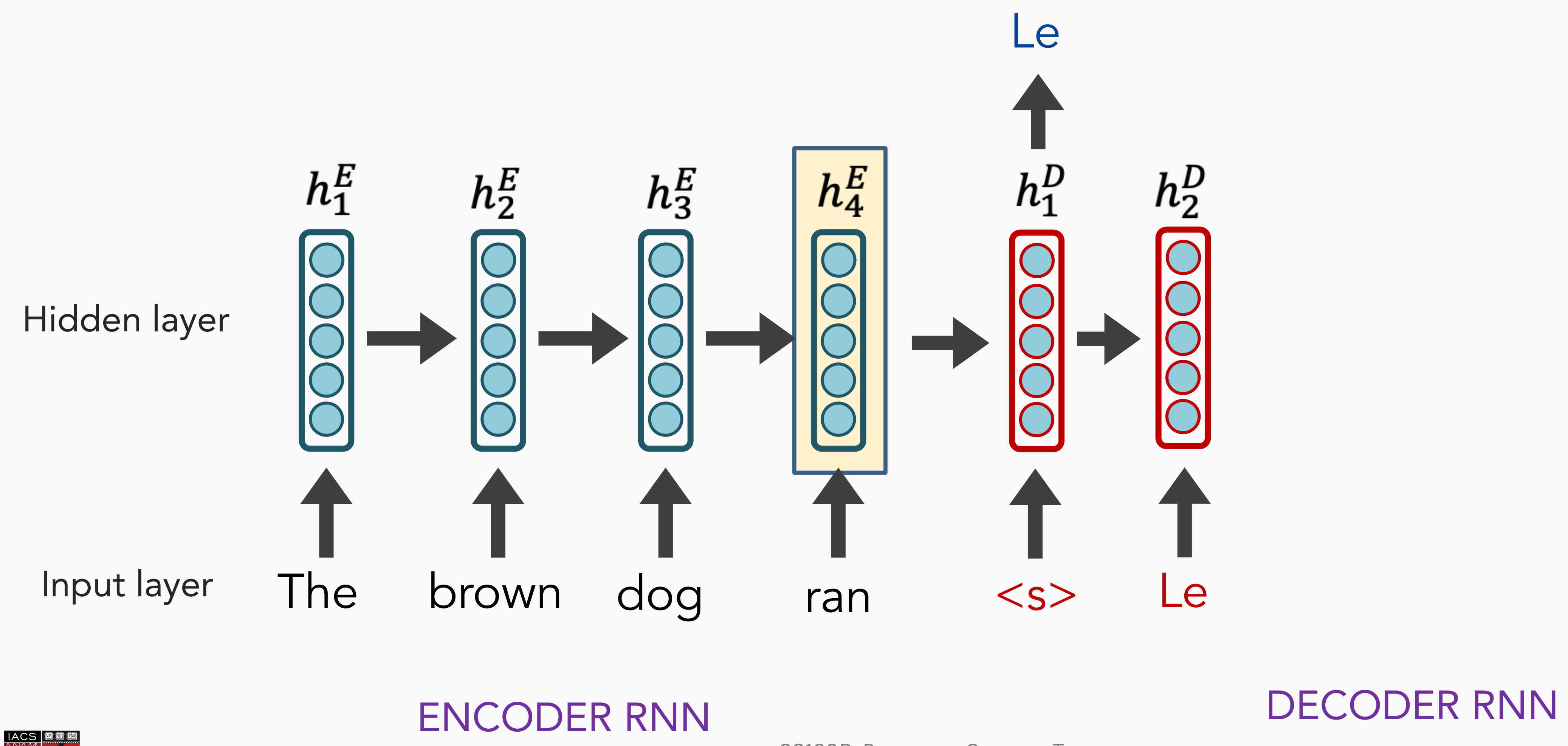

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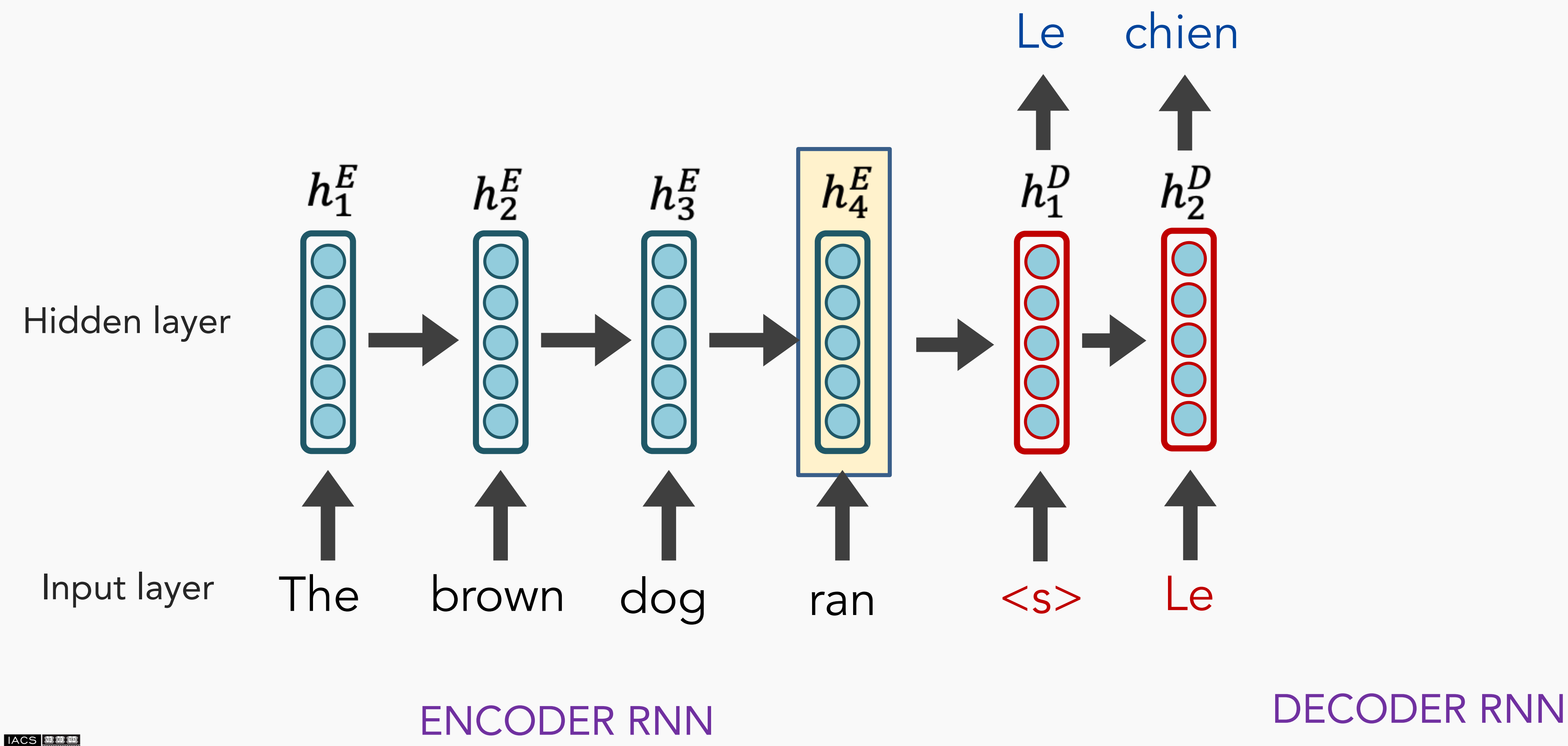

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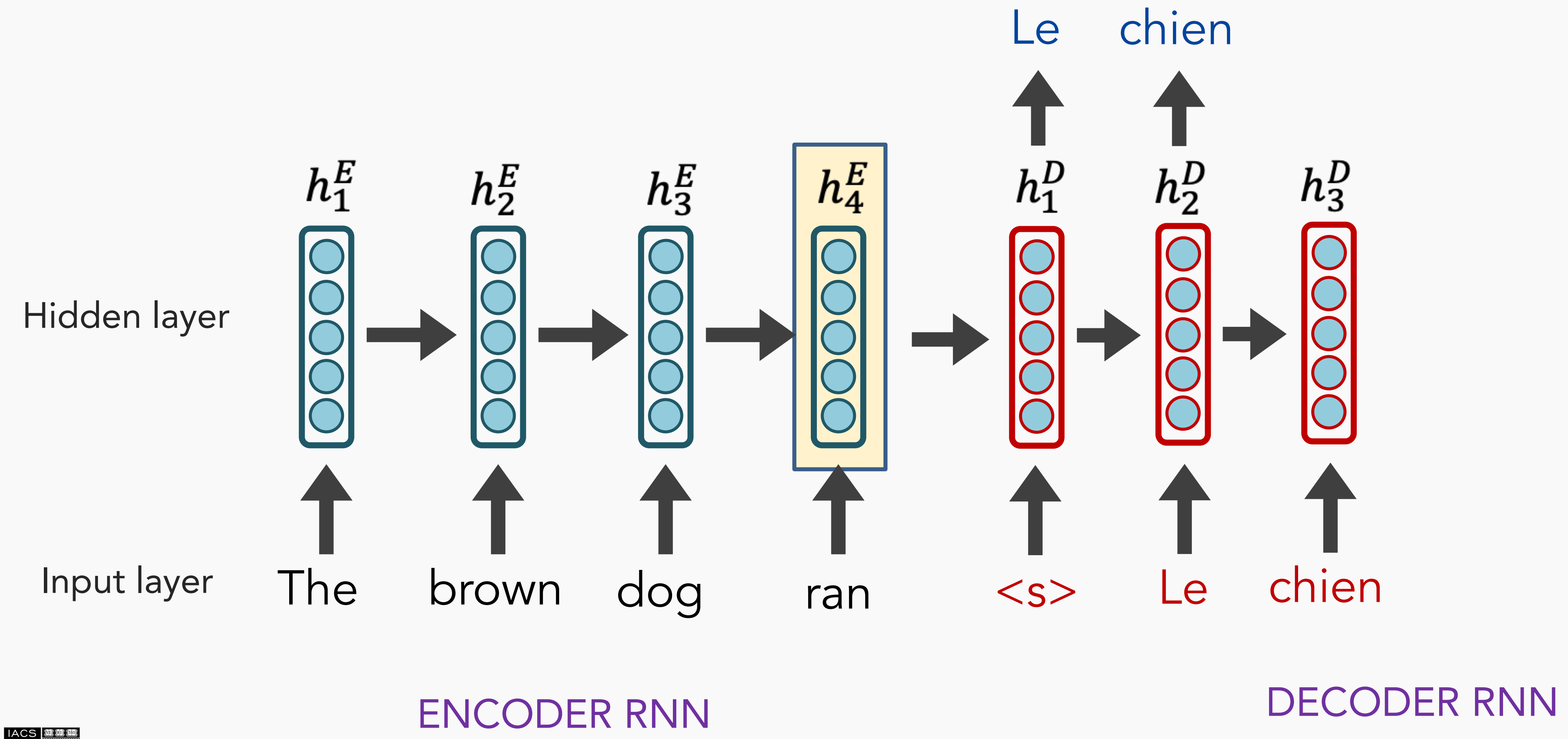

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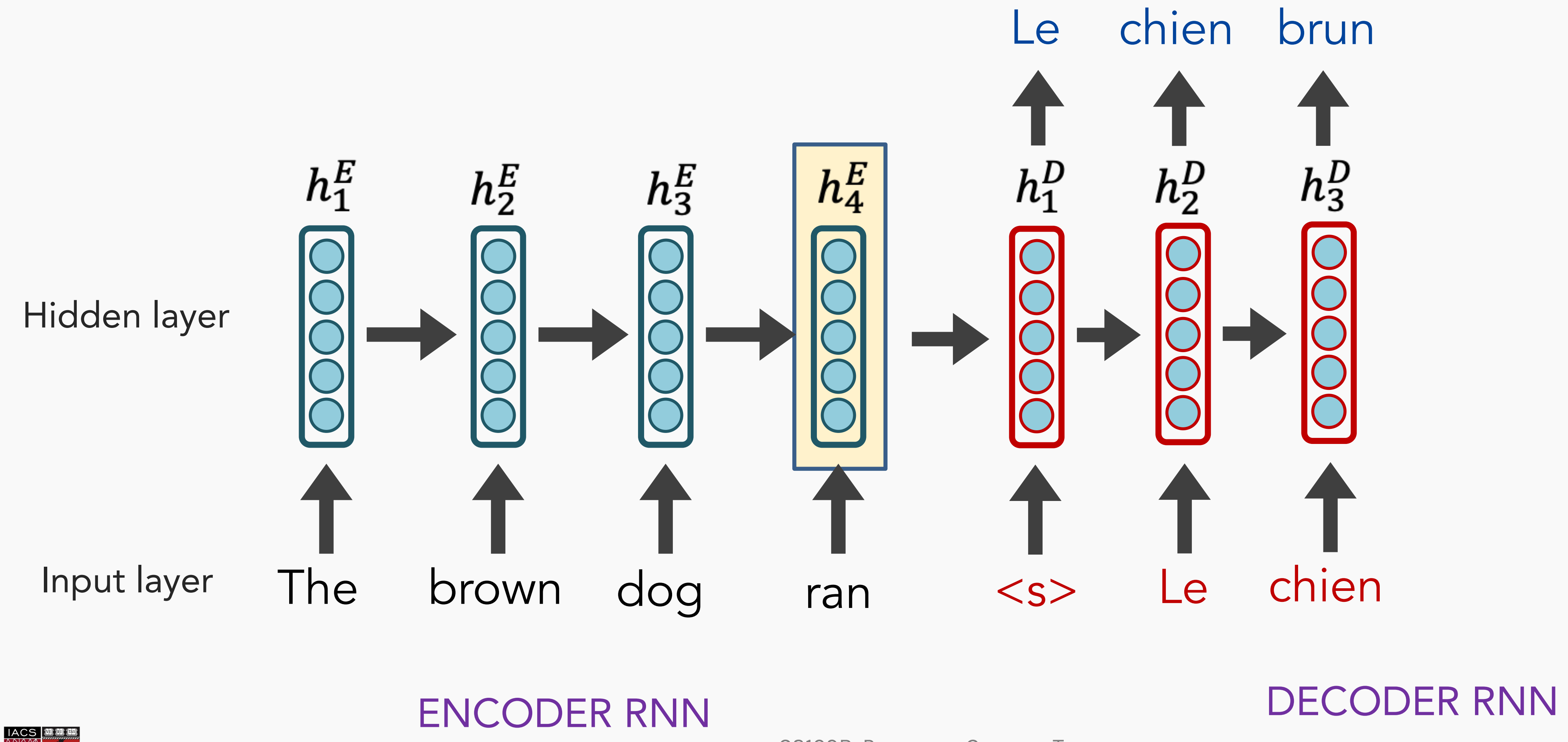

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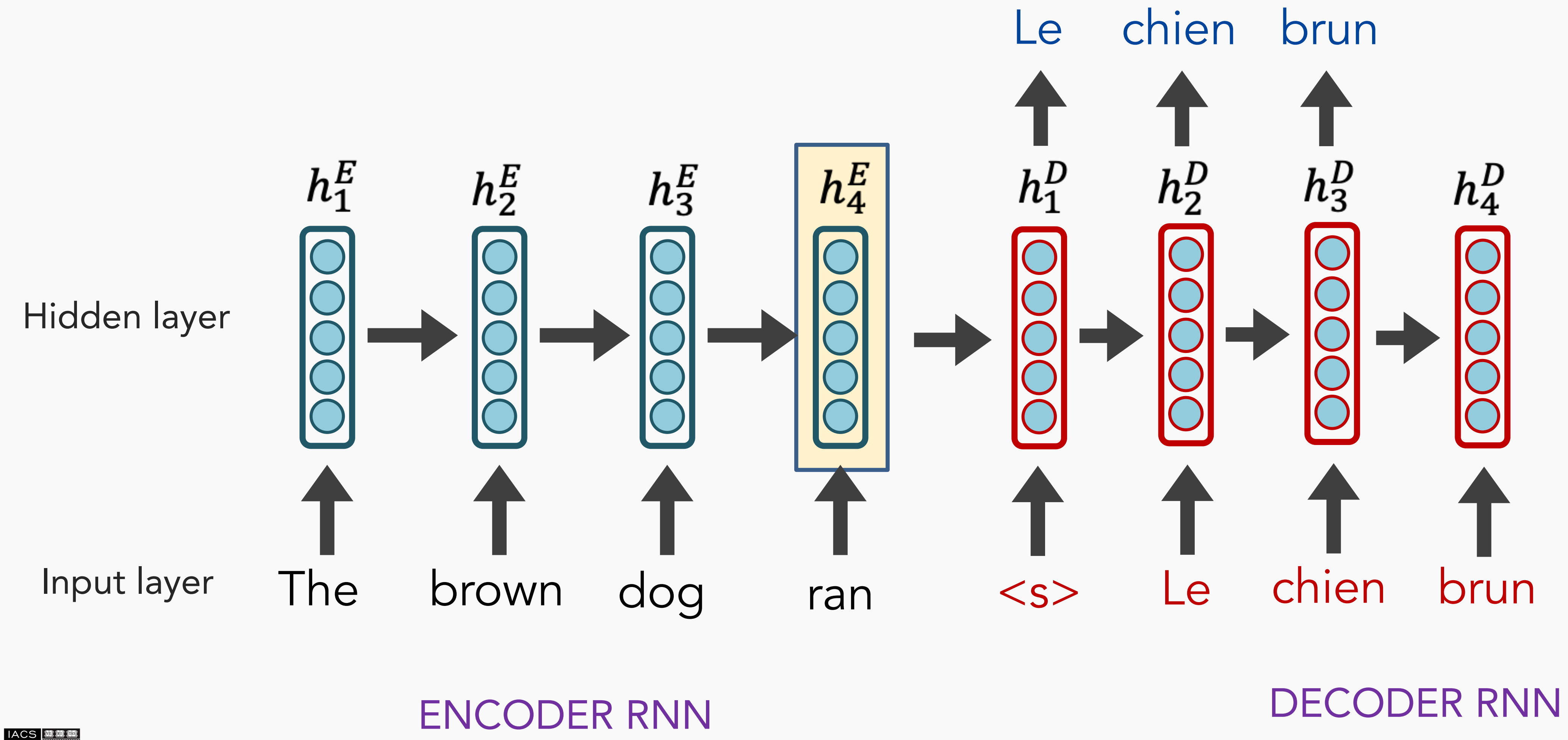

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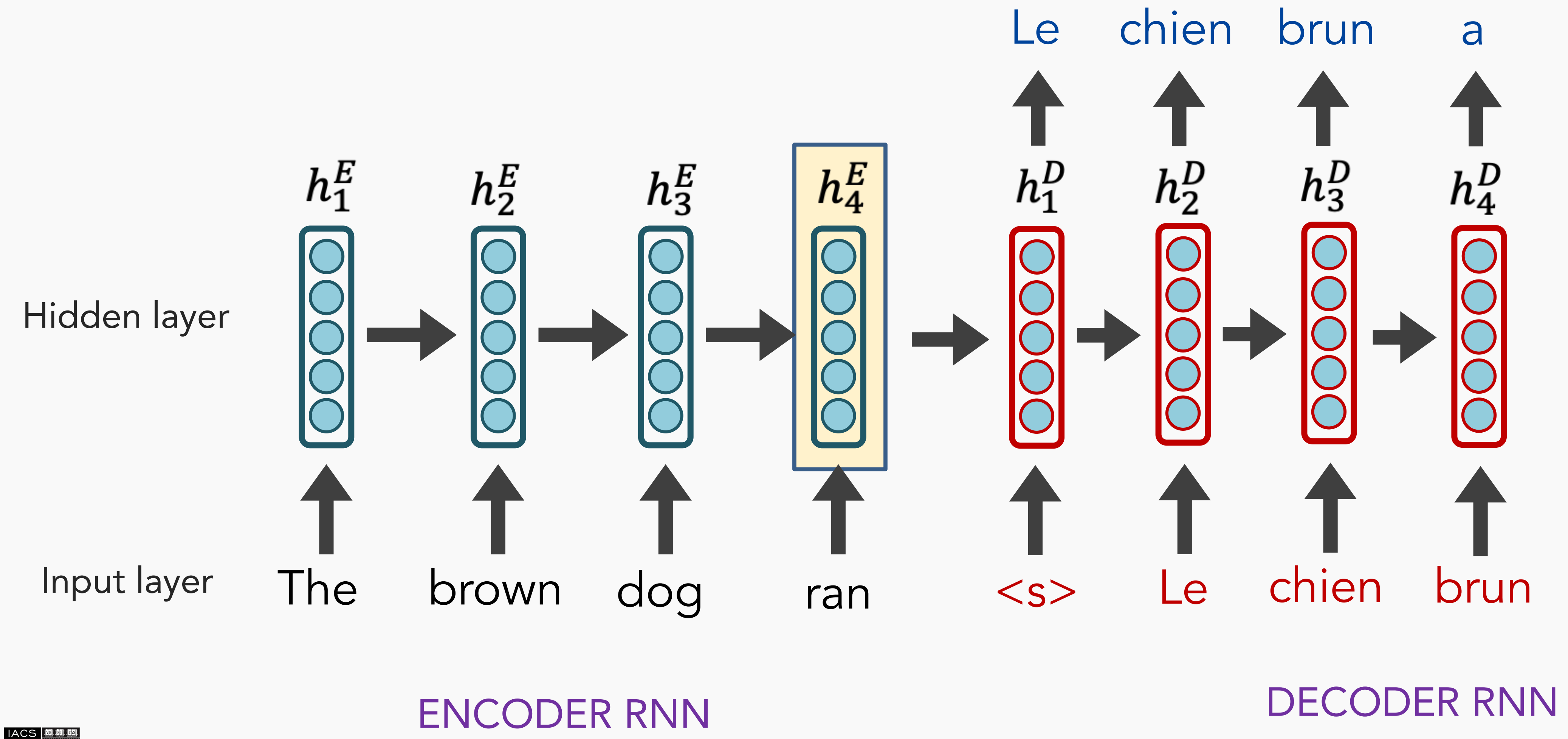

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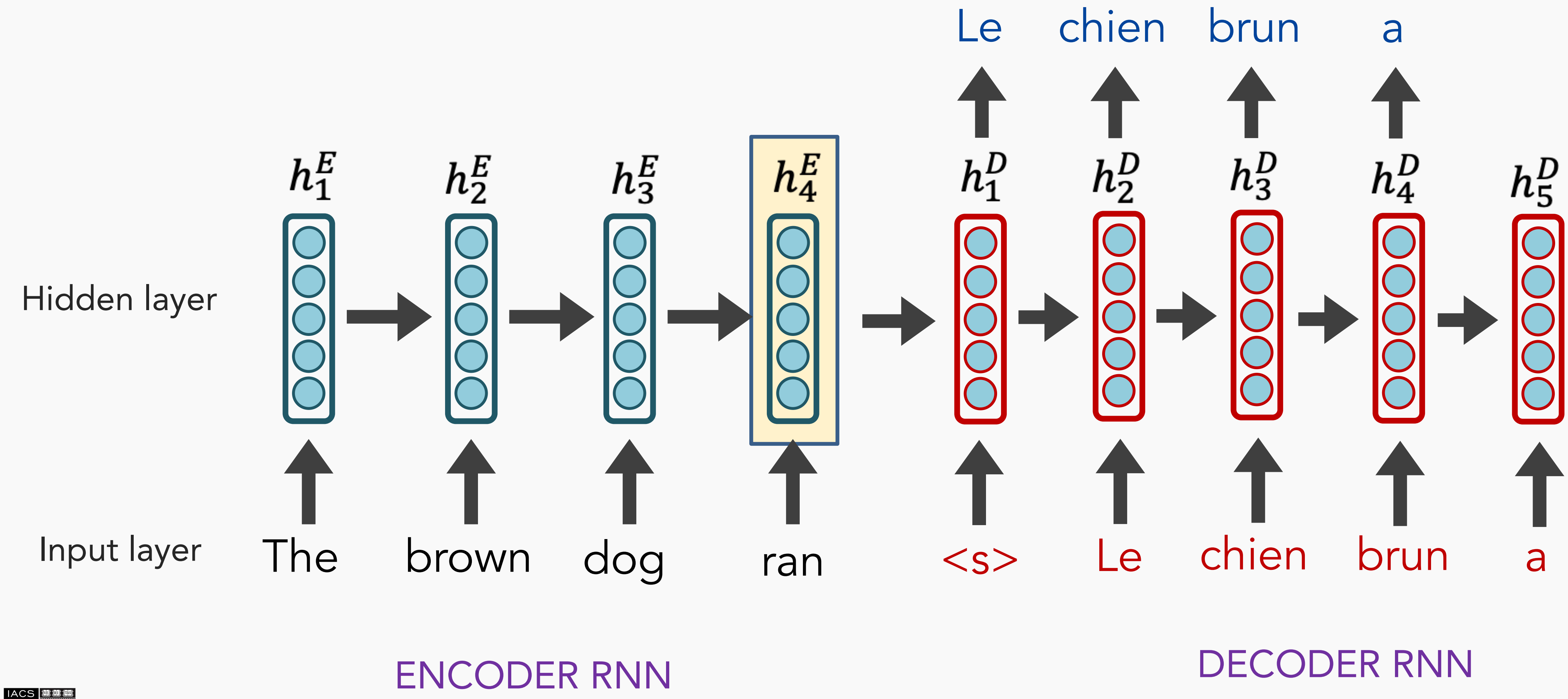

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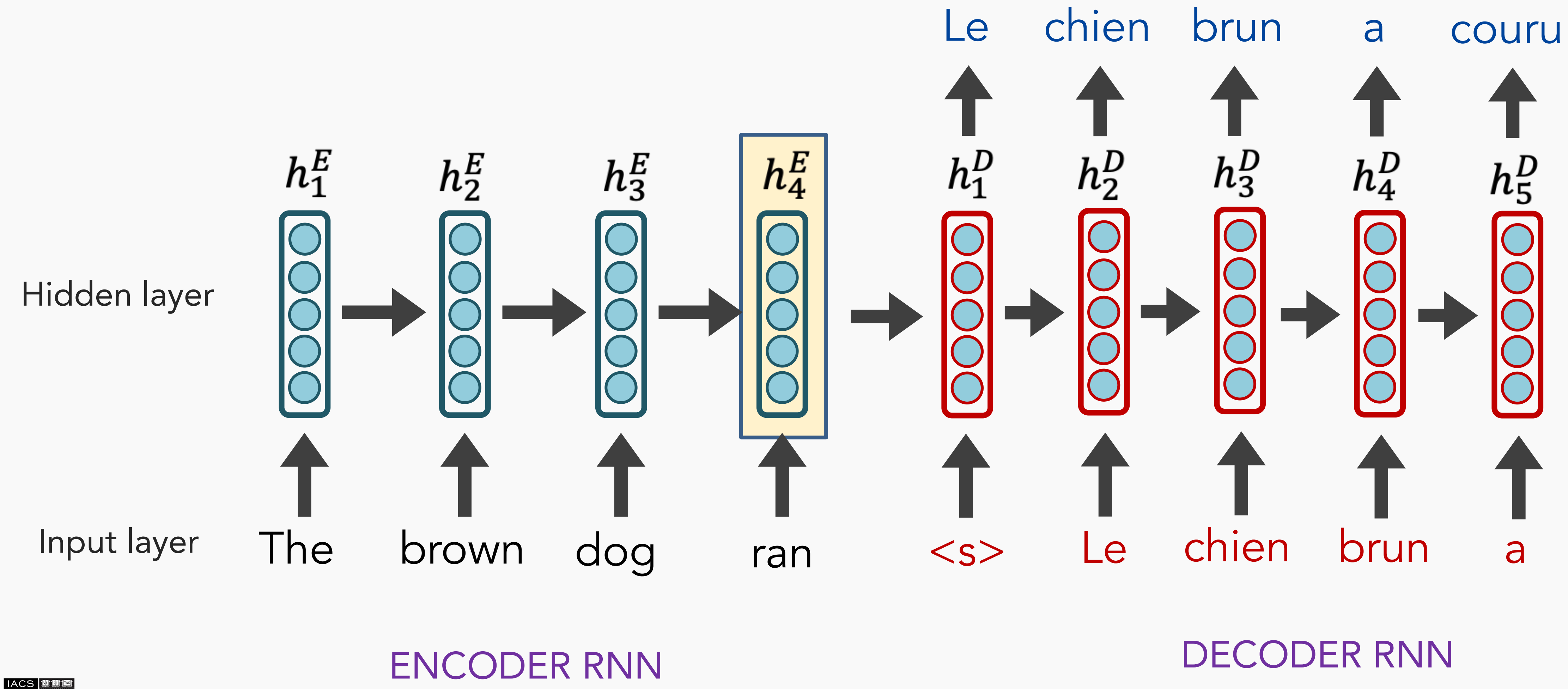

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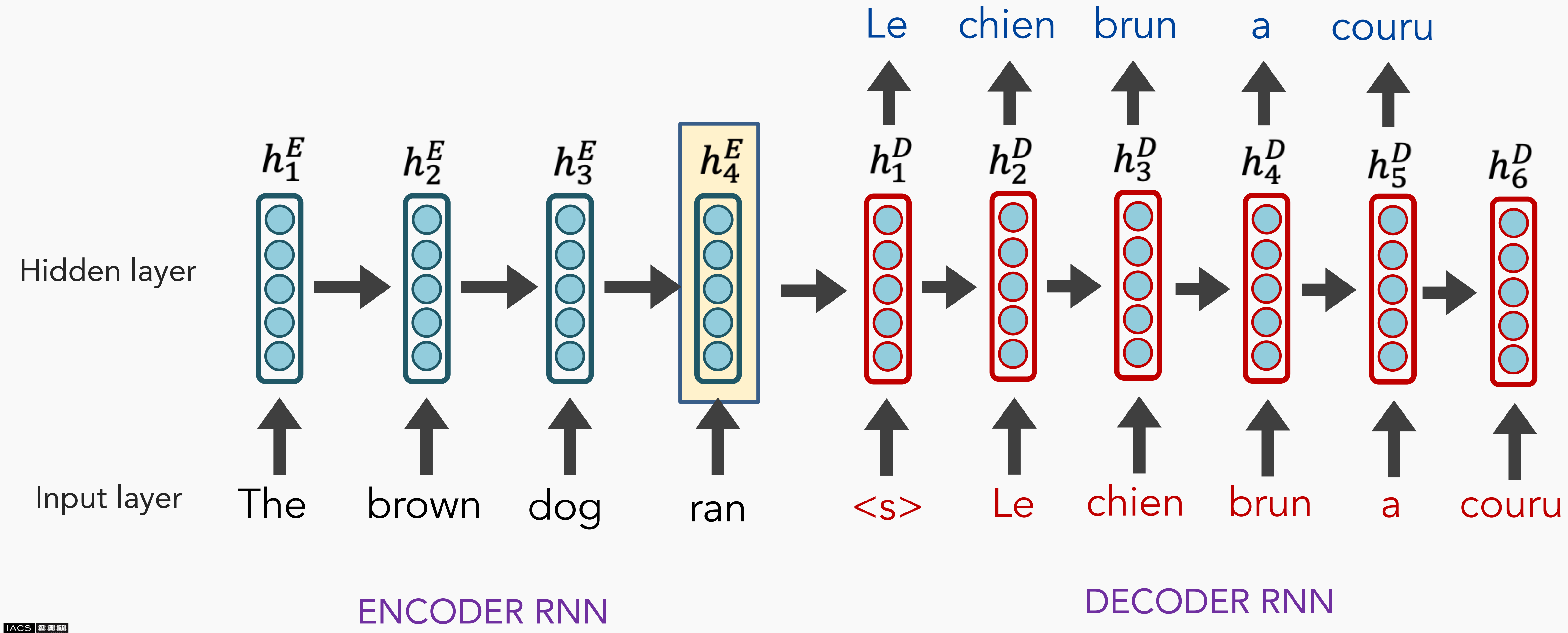

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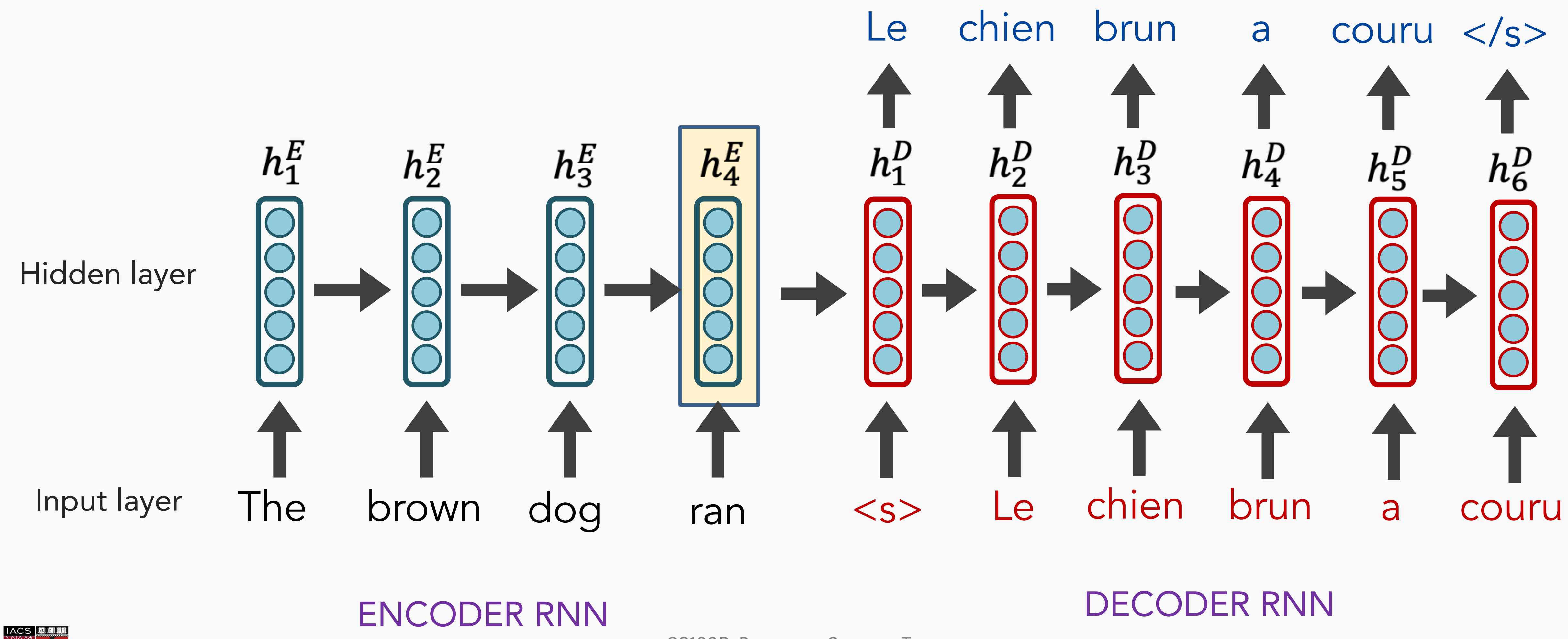

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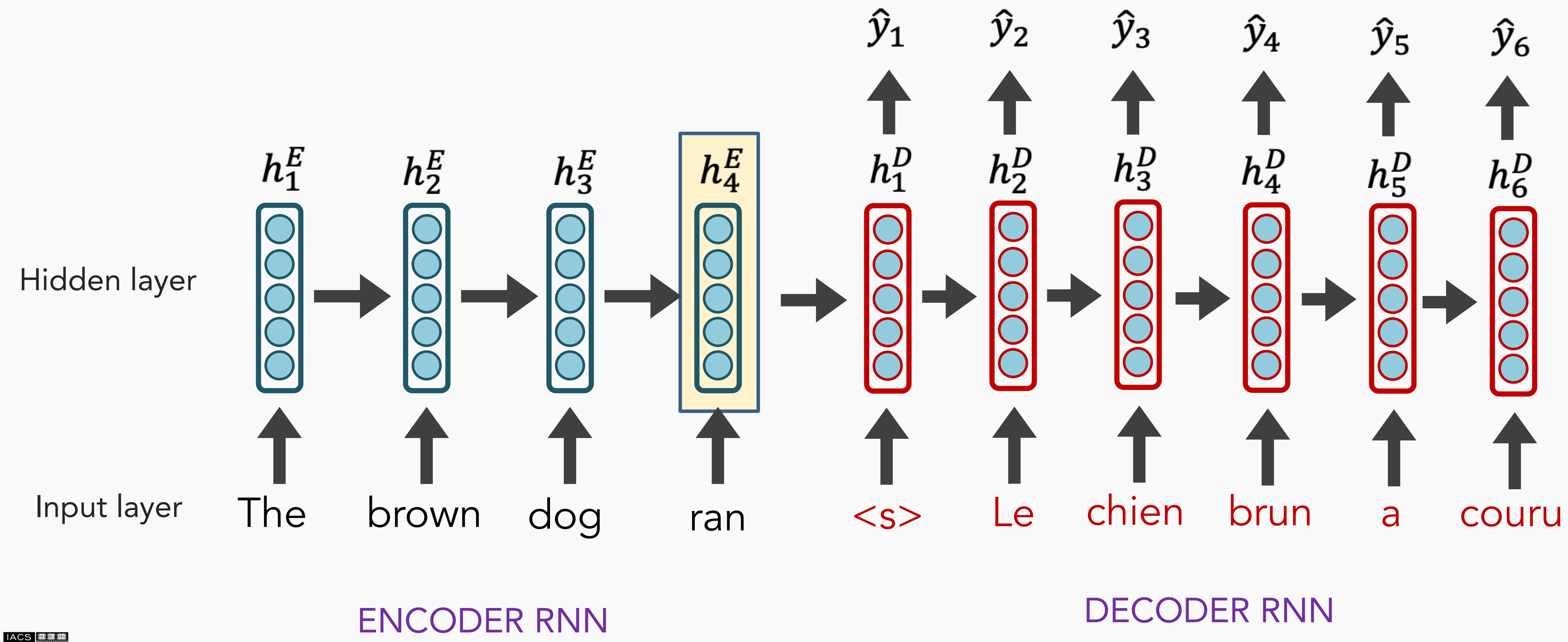

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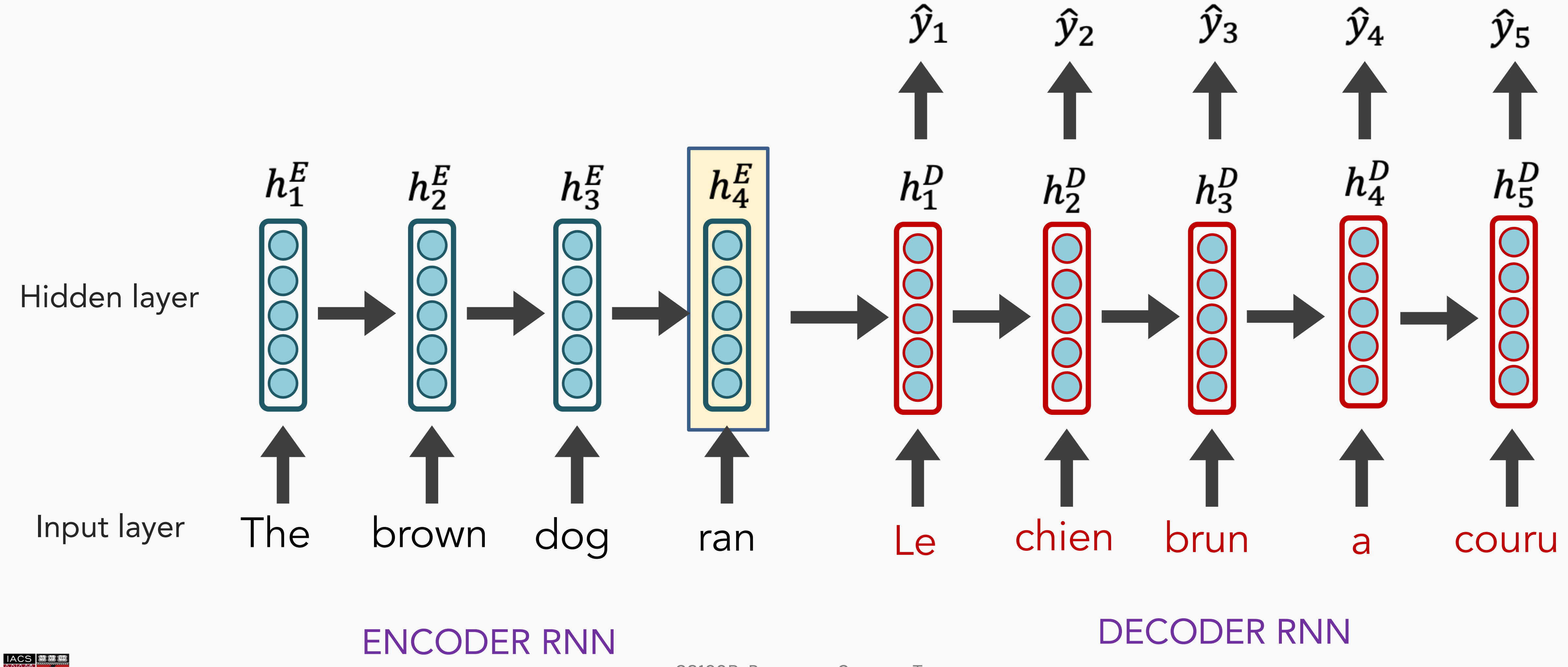
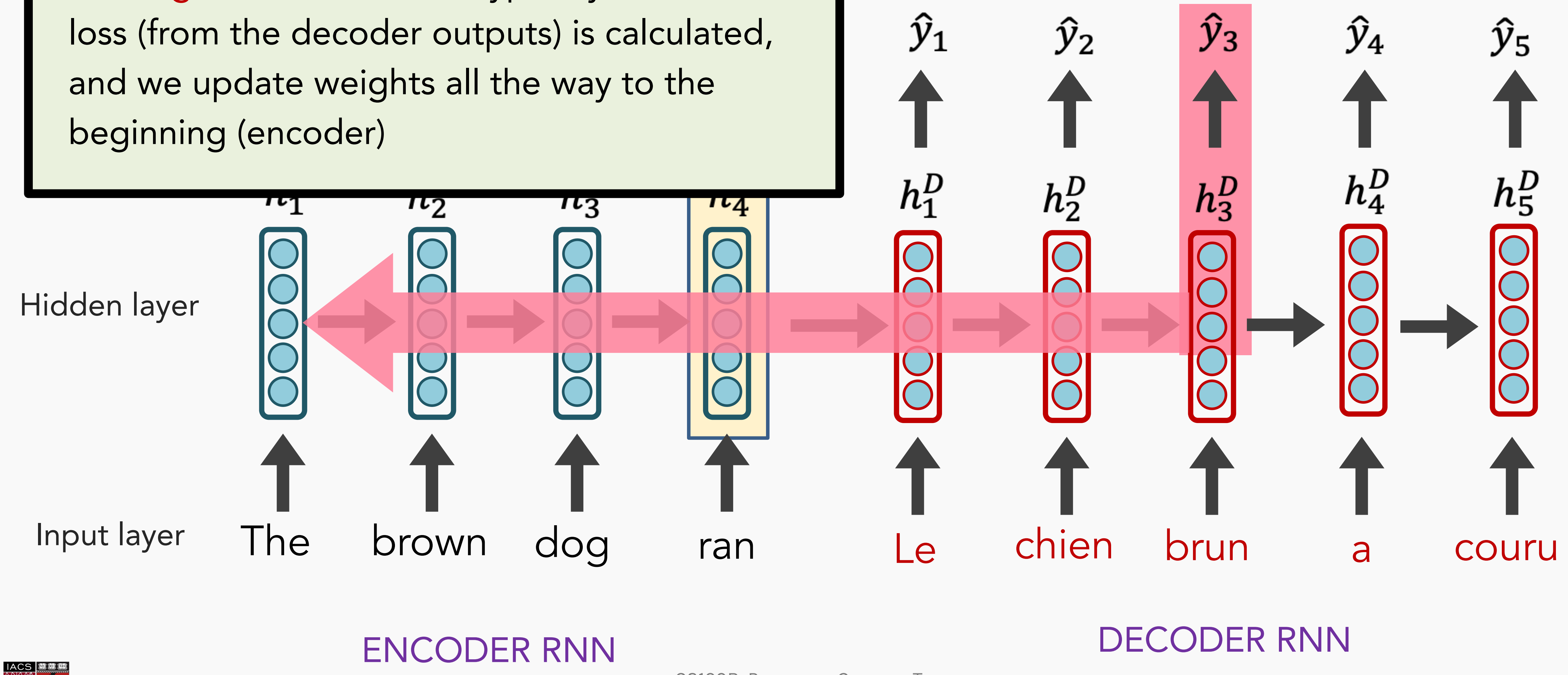


Sequence-to-Sequence (seq2seq)

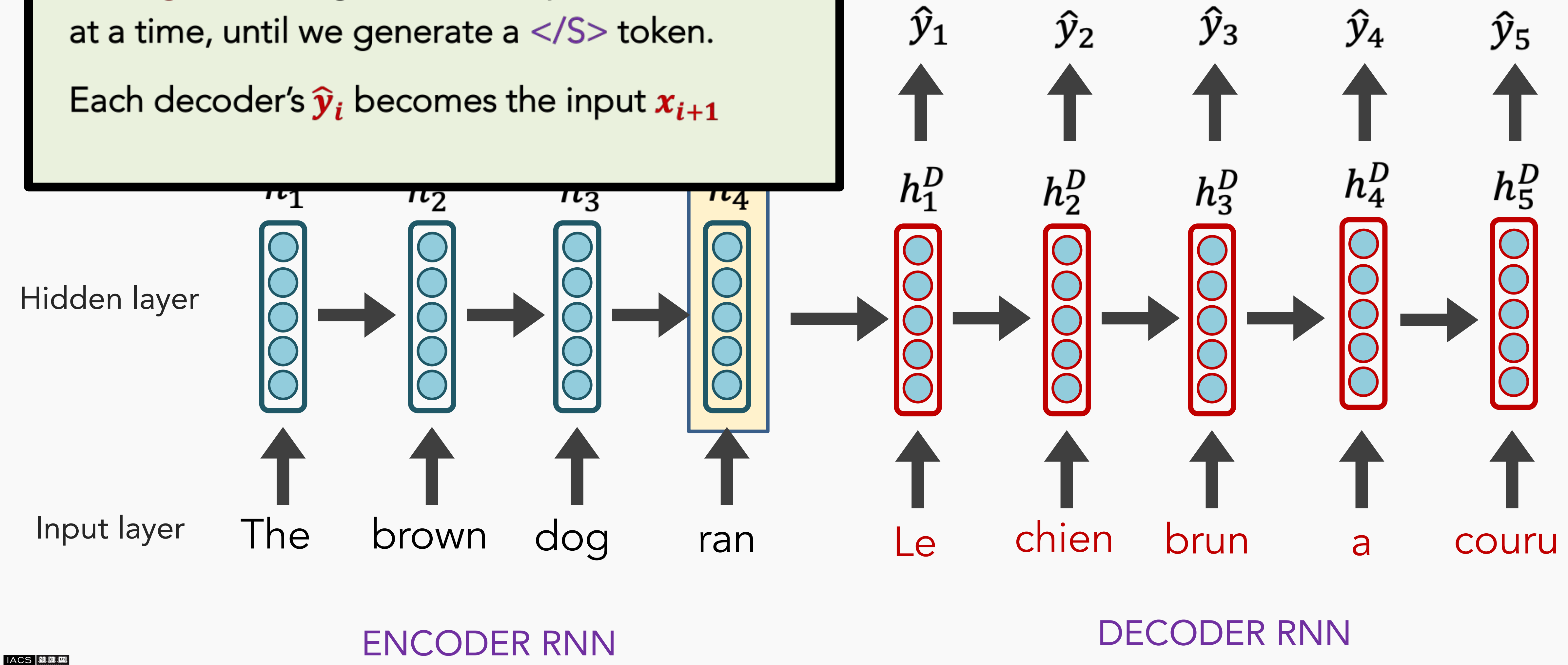
Training occurs like RNNs typically do; the loss (from the decoder outputs) is calculated, and we update weights all the way to the beginning (encoder)



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}

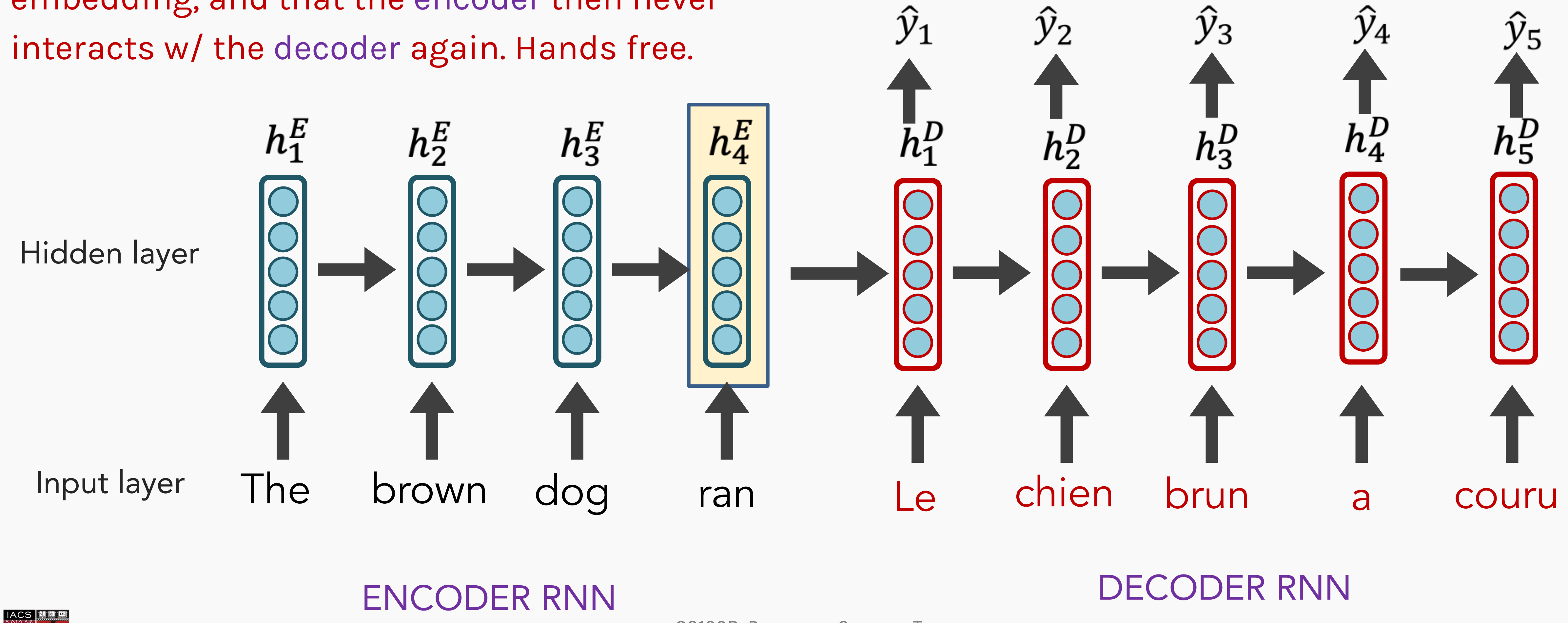


Sequence-to-Sequence (seq2seq)

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.

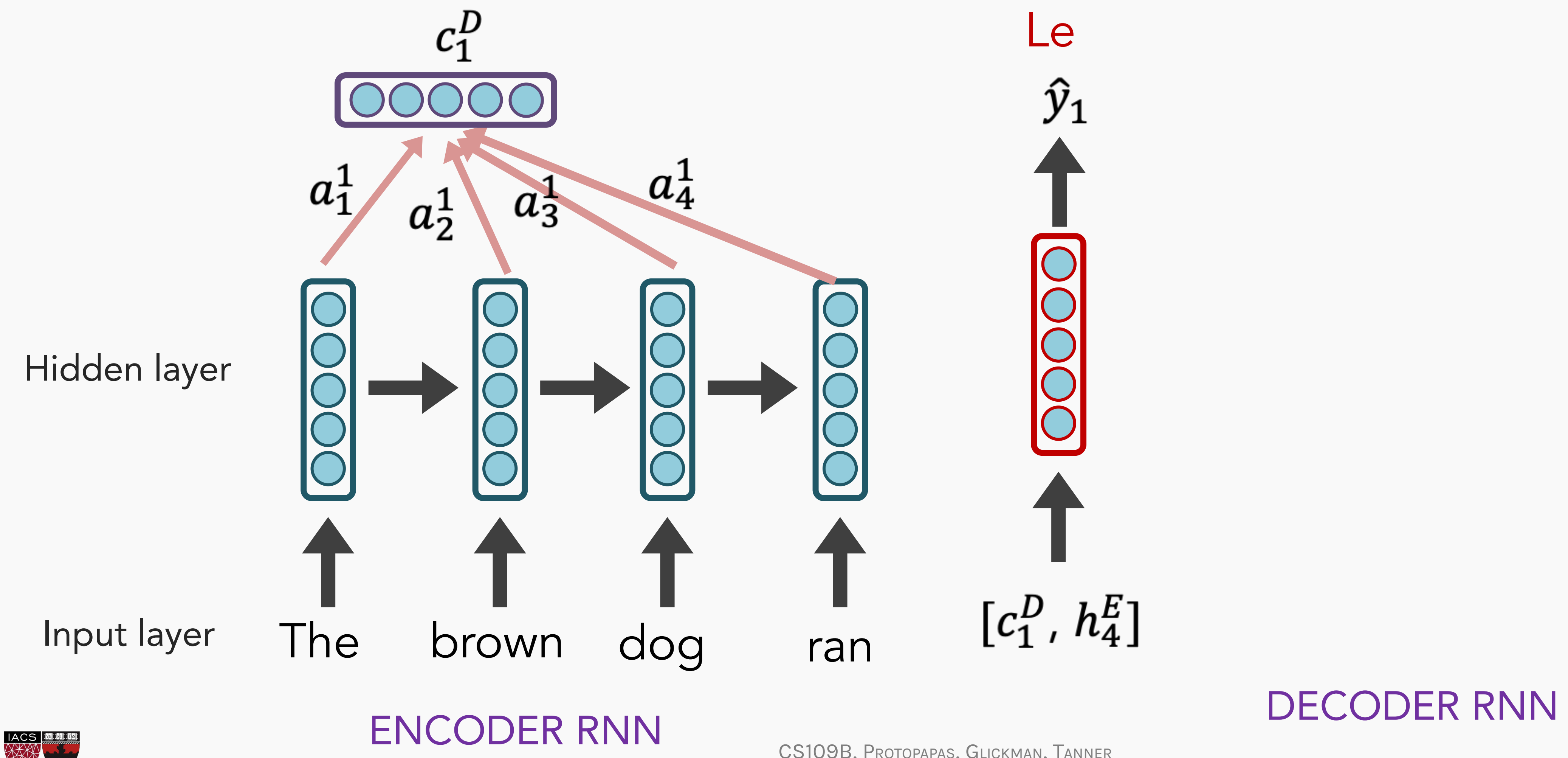


Sequence-to-Sequence (seq2seq)

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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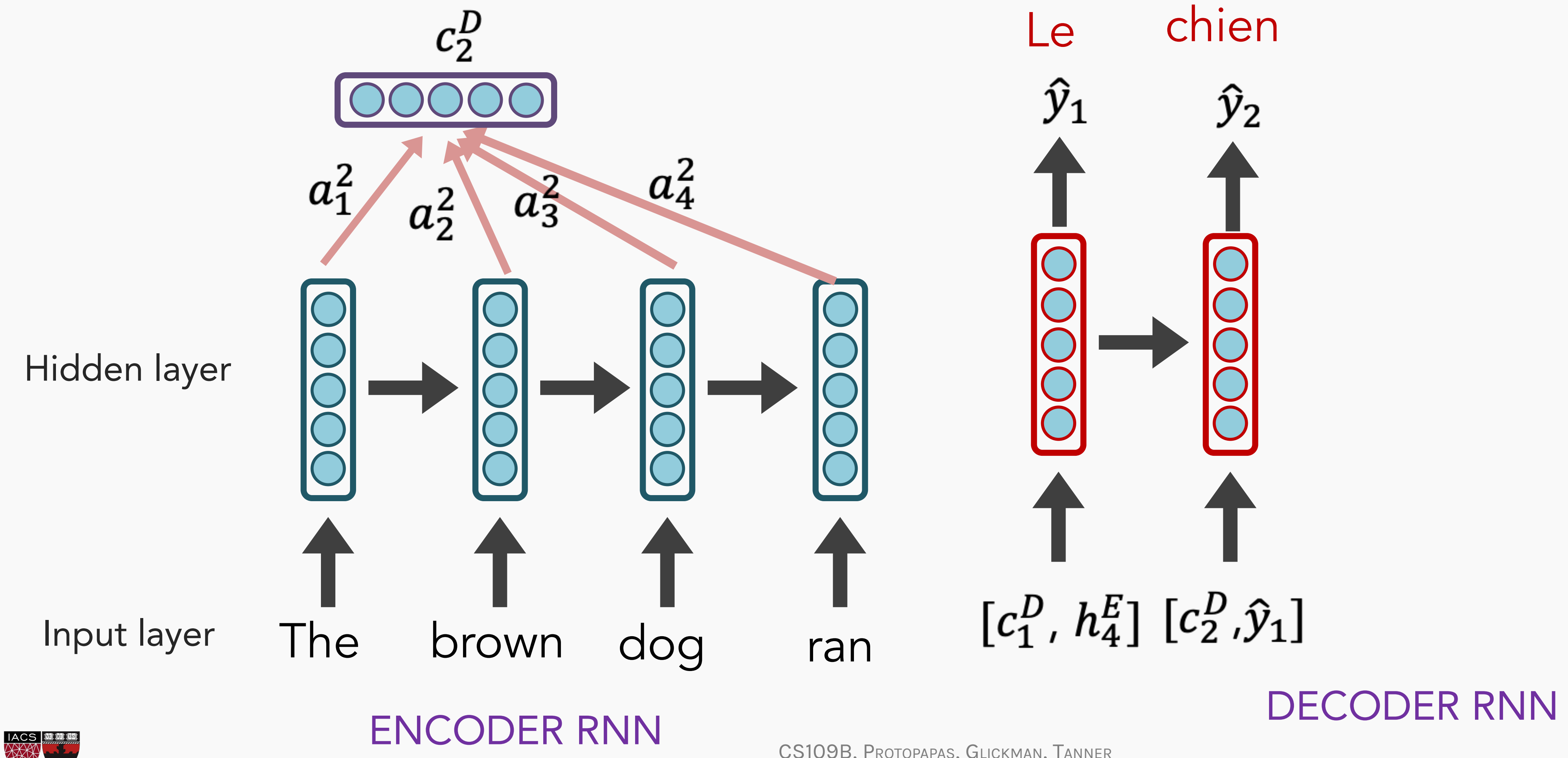

seq2seq + Attention

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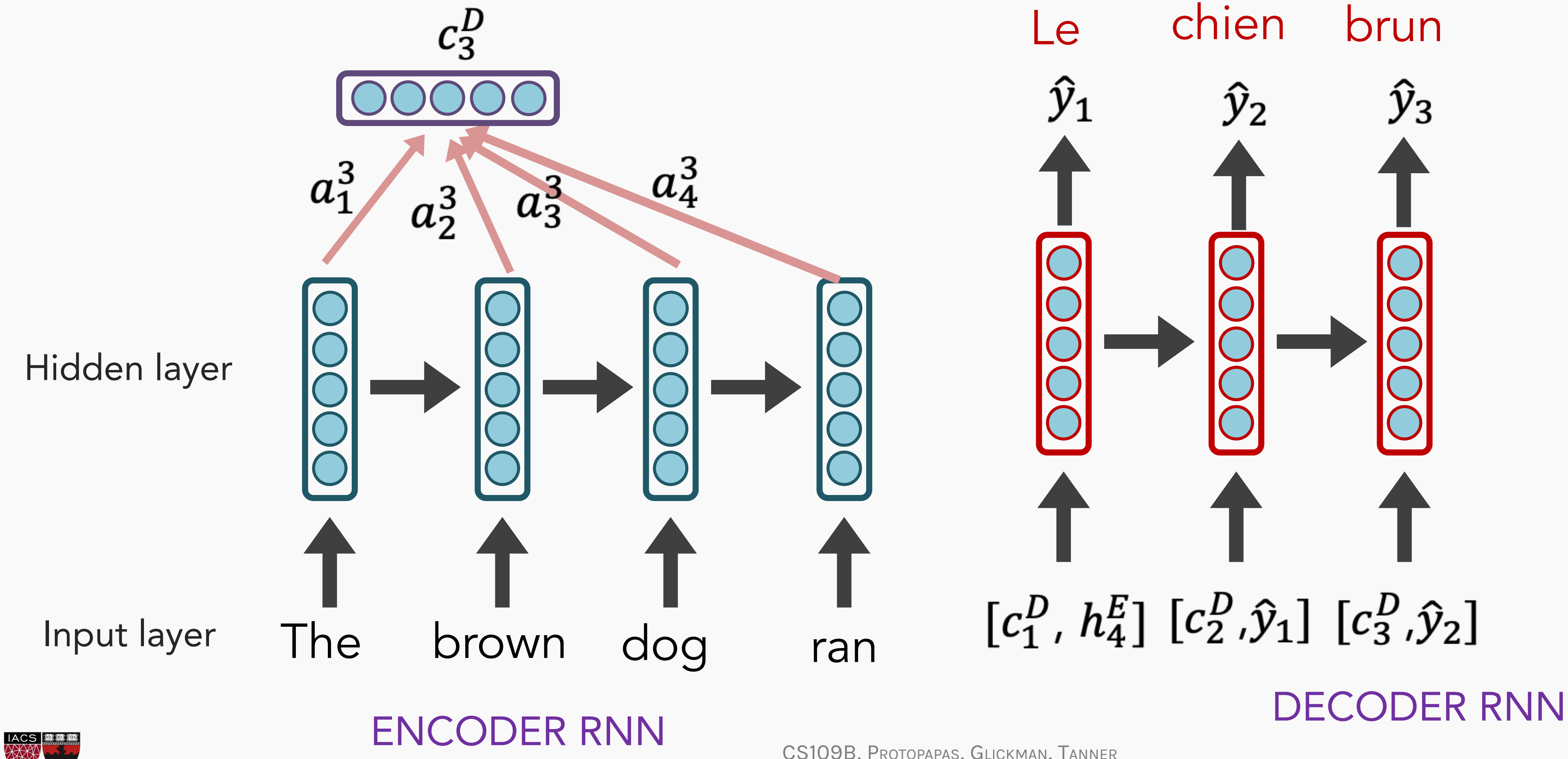

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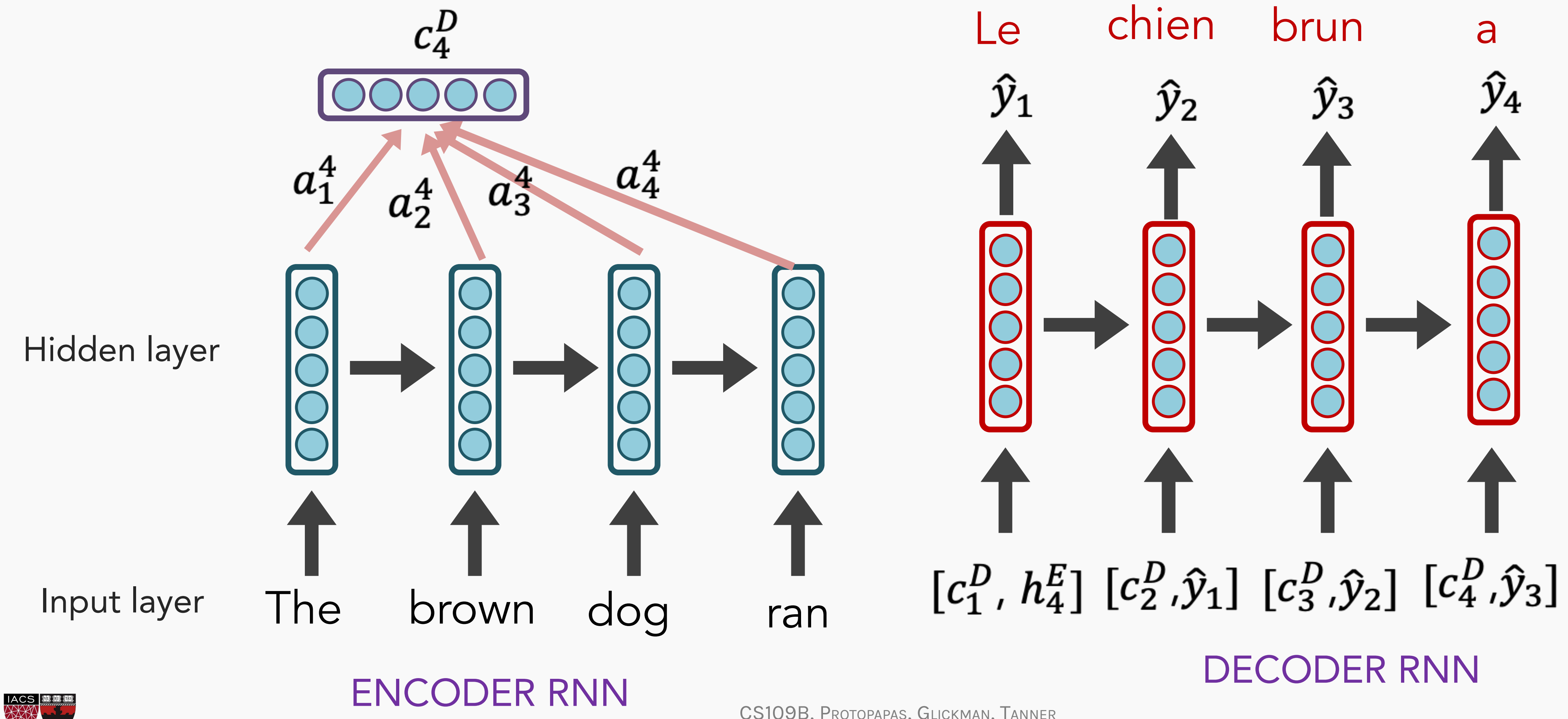

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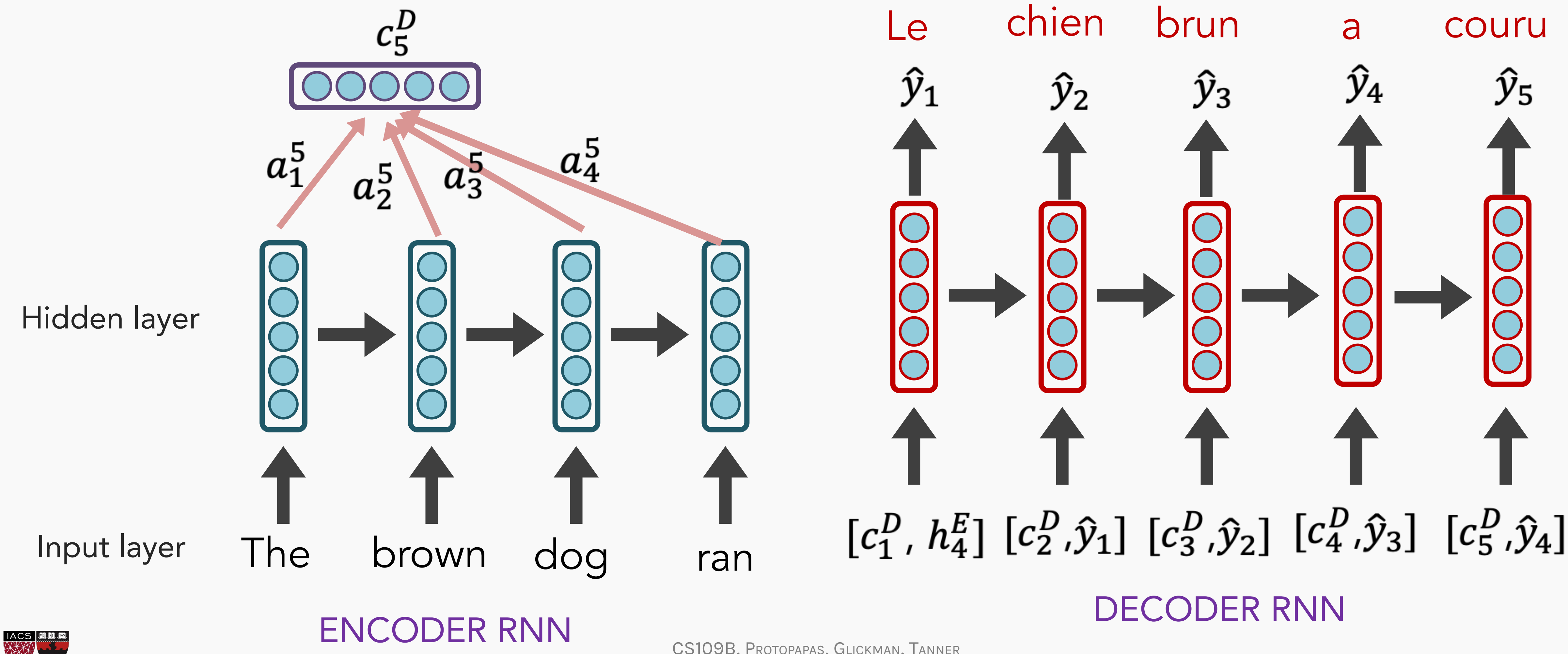


seq2seq + Attention

Attention:

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

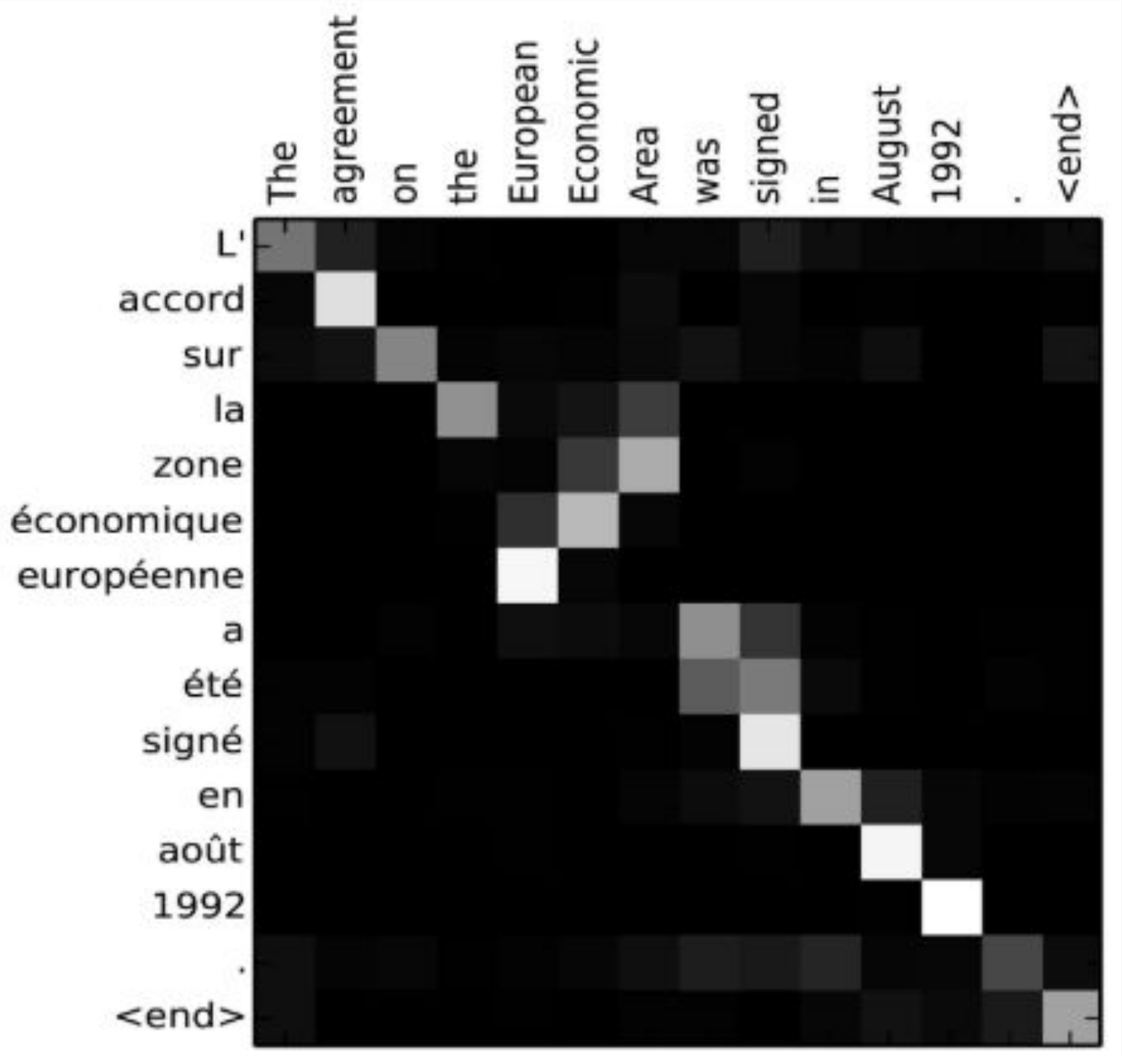


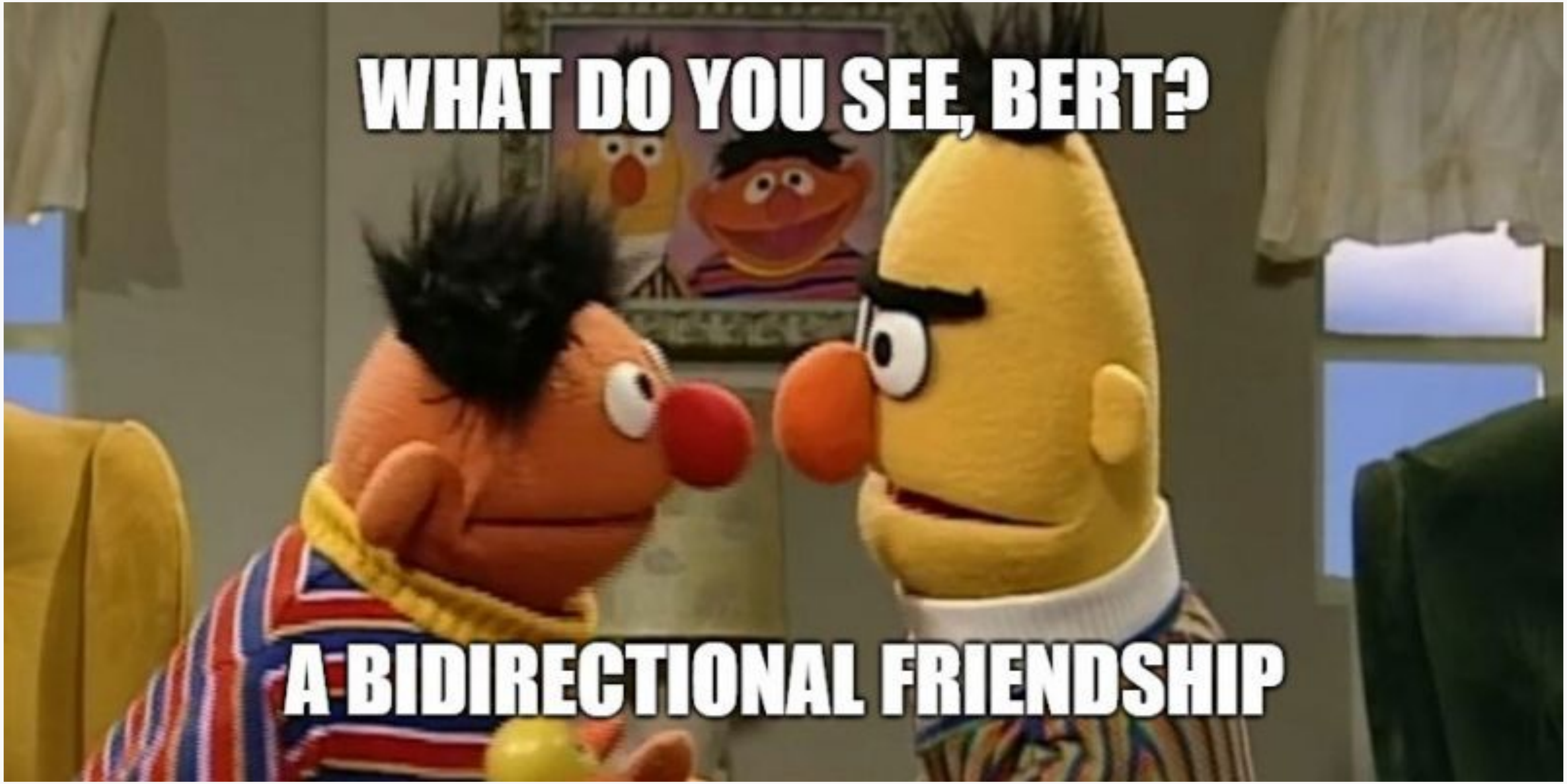
Image source: Fig 3 in [Bahdanau et al., 2015]

Outline

- Seq2Seq +Attention

- **Transformers +BERT**

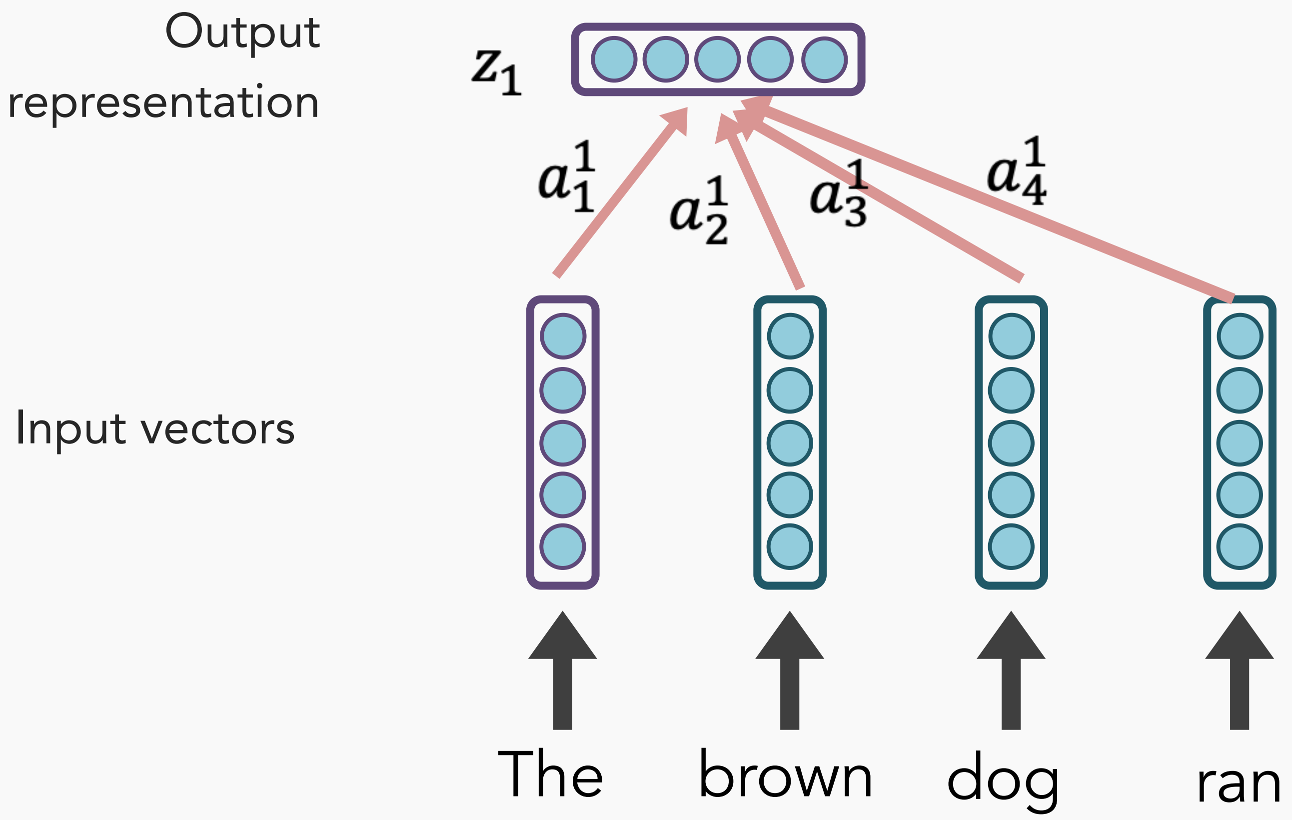
- Embeddings


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

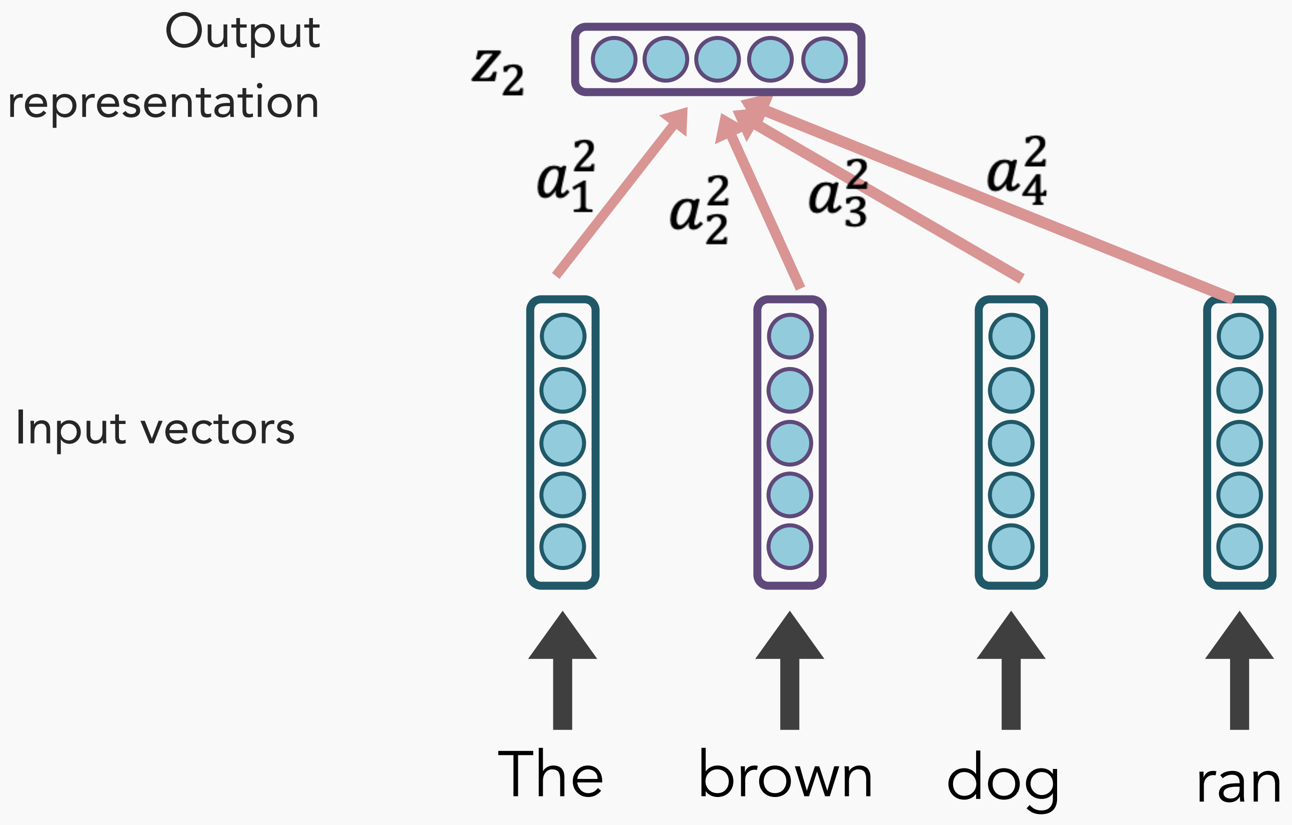
Self-Attention



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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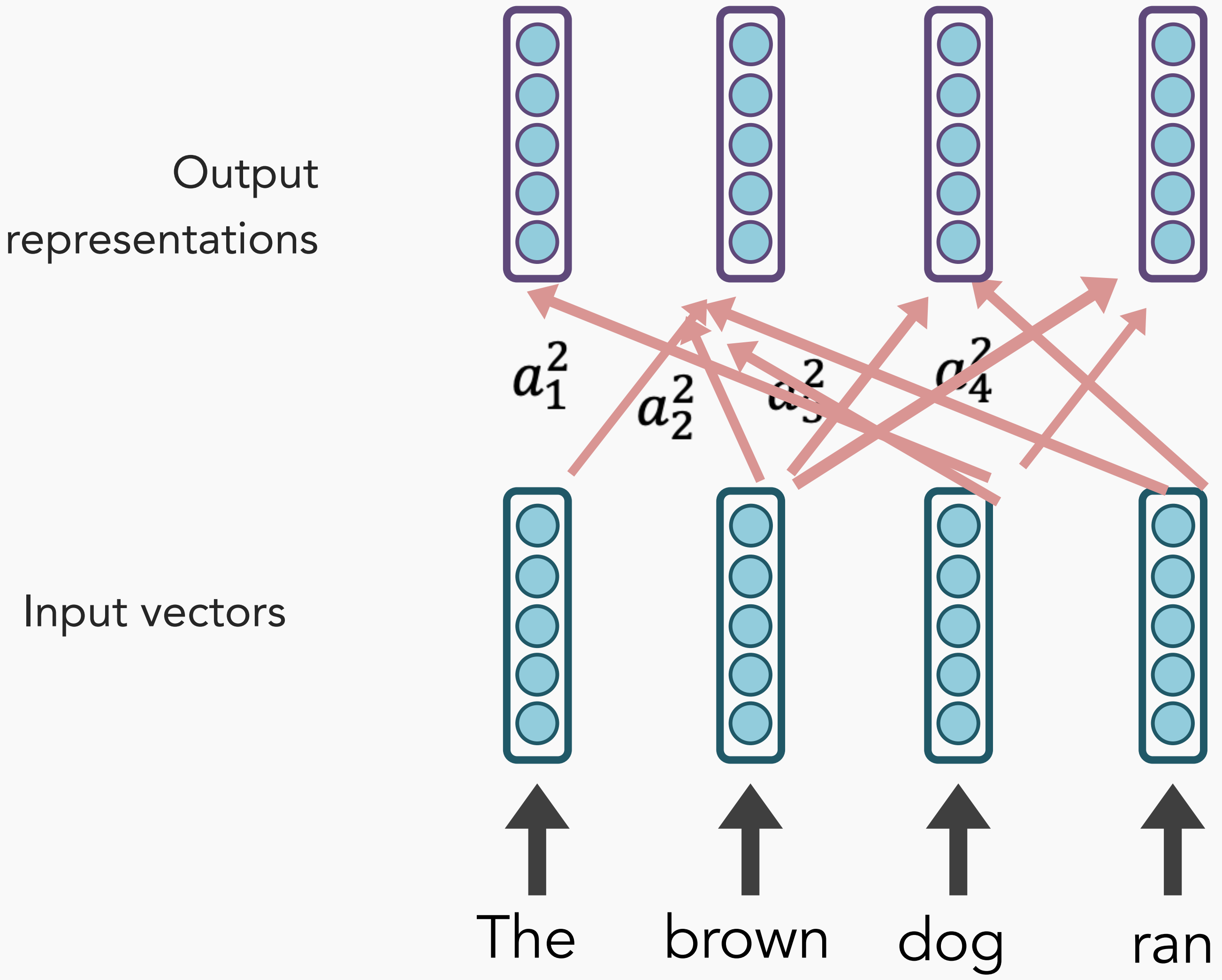
Self-Attention



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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

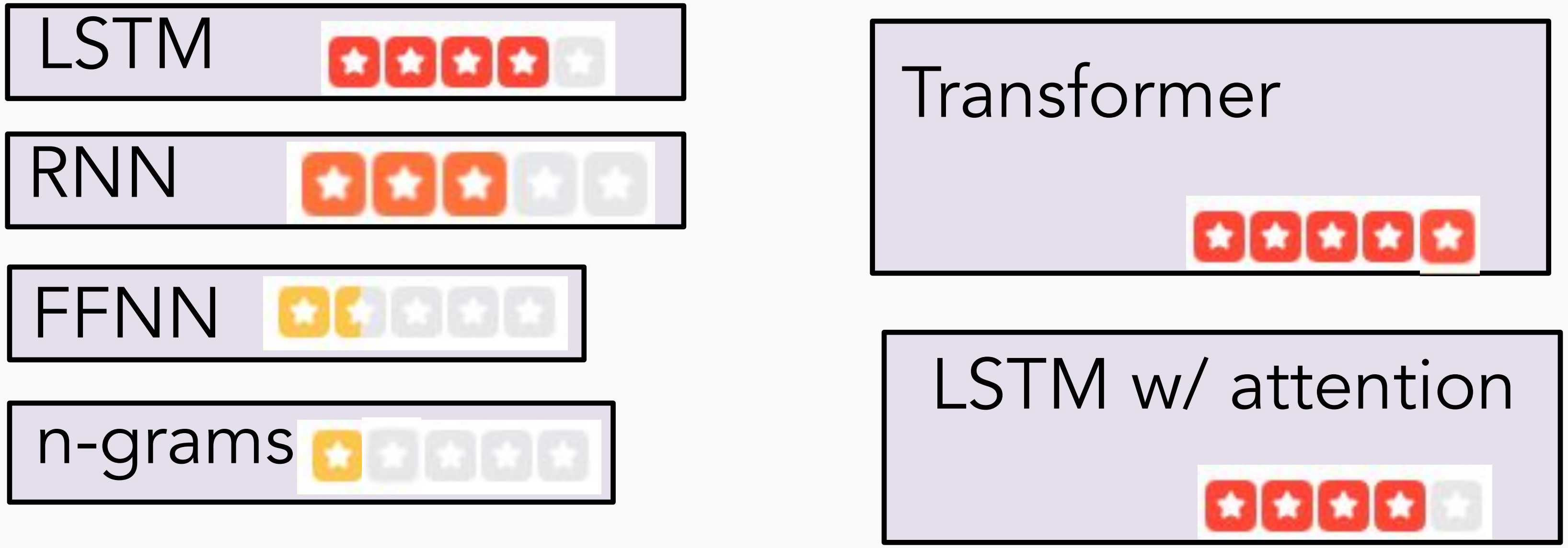
- There has been significant progress in the past few years.
- Some of the complex models are incredible, but rely on having a lot of data and computational resources (e.g., Transformers)
- With all data science and machine learning, it's best to understand your data and your task very well, then clean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

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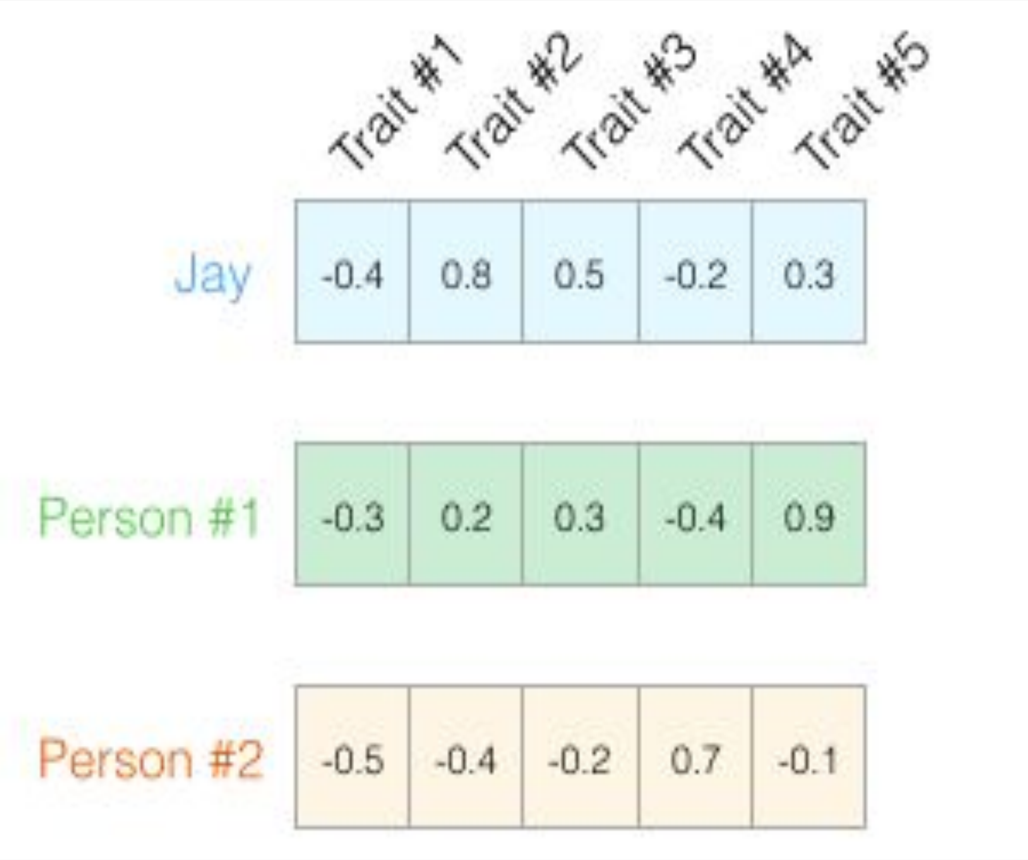
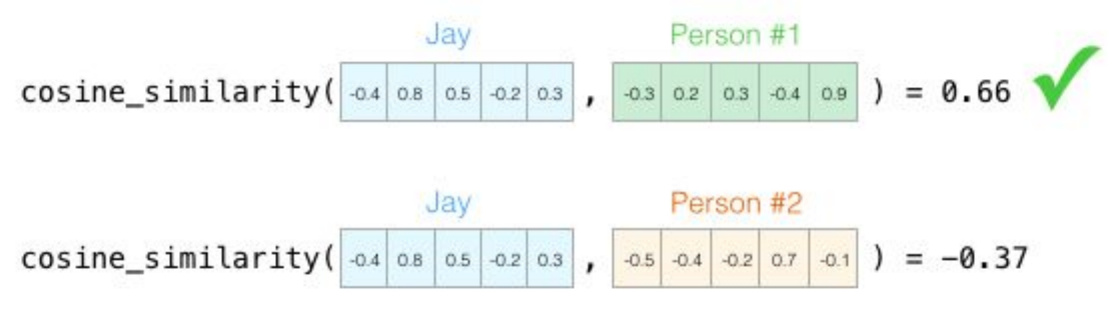
- Transformers +BERT
- **Embeddings**

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.

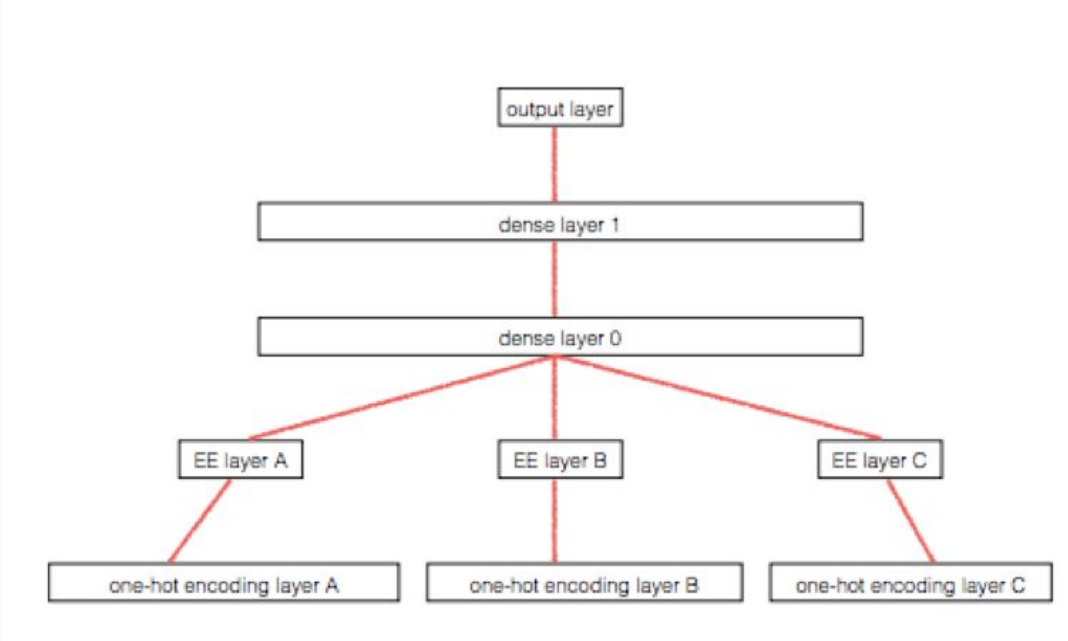
We usually **one-hot encode** this: a single store is a length 3000 bit-vector with one bit flipped on.

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)

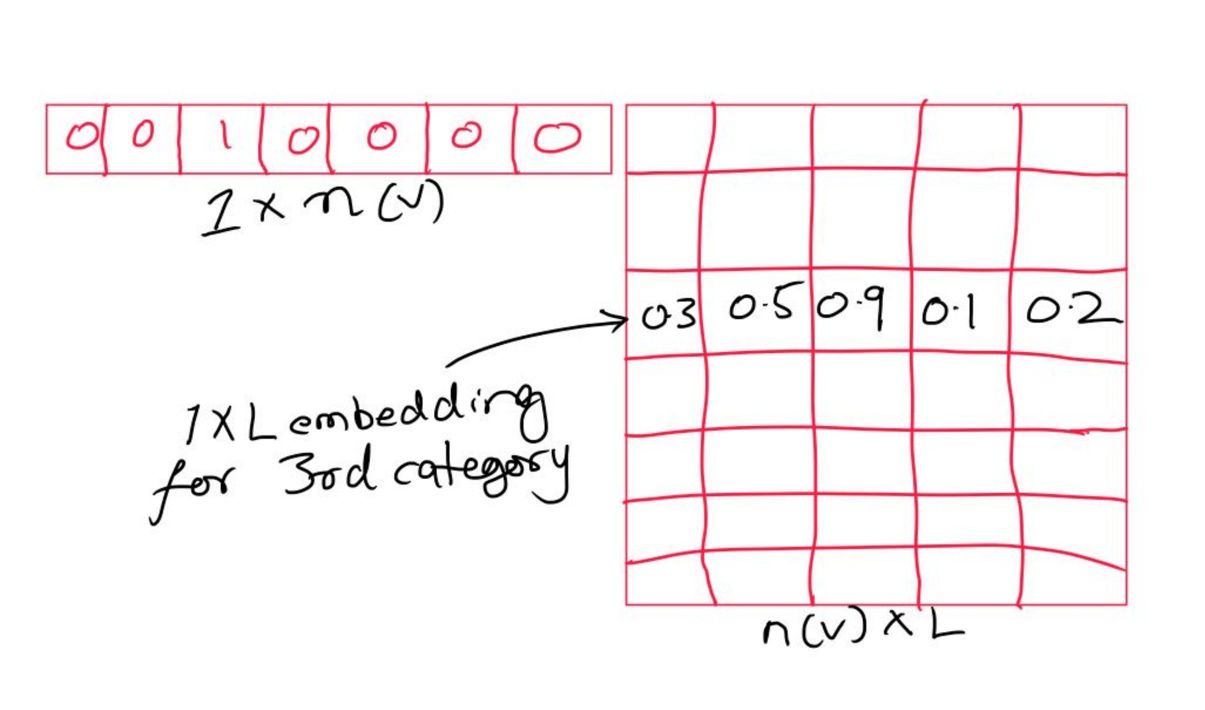
A 1-hot vector for a categorical variable with cardinality can be written using the Kronecker Delta symbol as:

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

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.

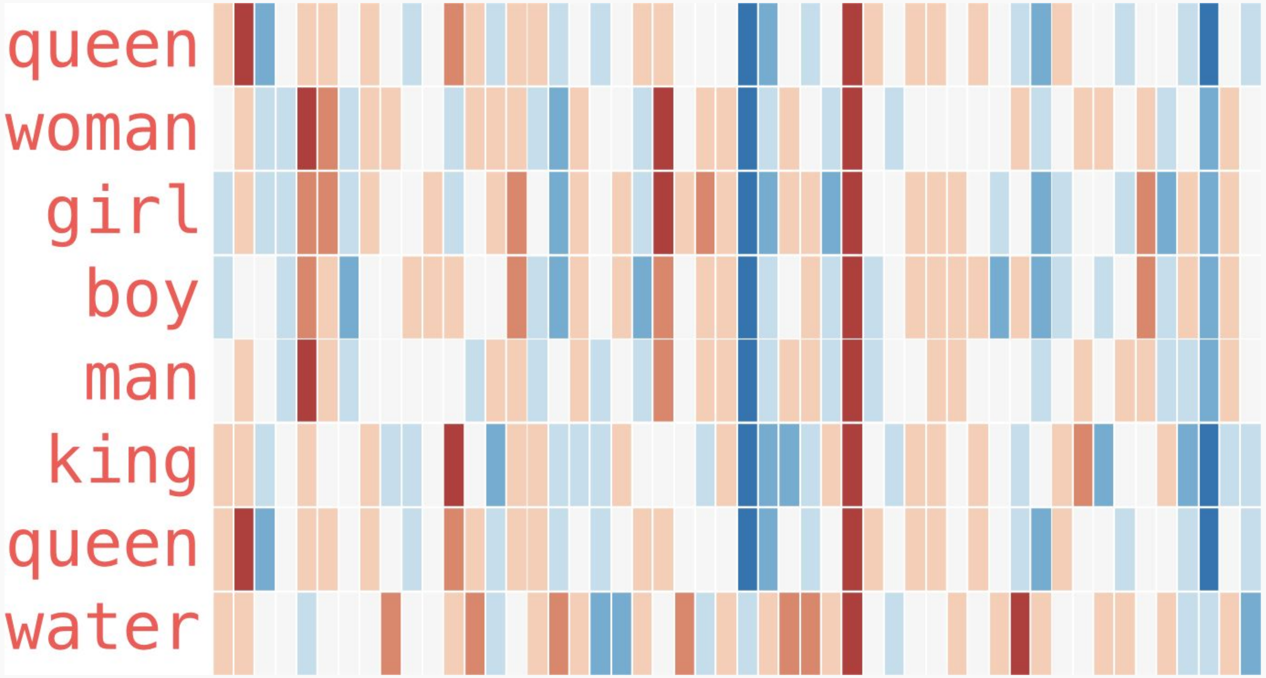
```python
def embedding_input(emb_name, n_items, n_fact=20, l2regularizer=1e-4):
    inp = Input(shape=(1,), dtype='int64', name=emb_name)
    return inp, Embedding(n_items, n_fact, input_length=1, embeddings_regularizer=l2(l2regularizer))(inp)

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

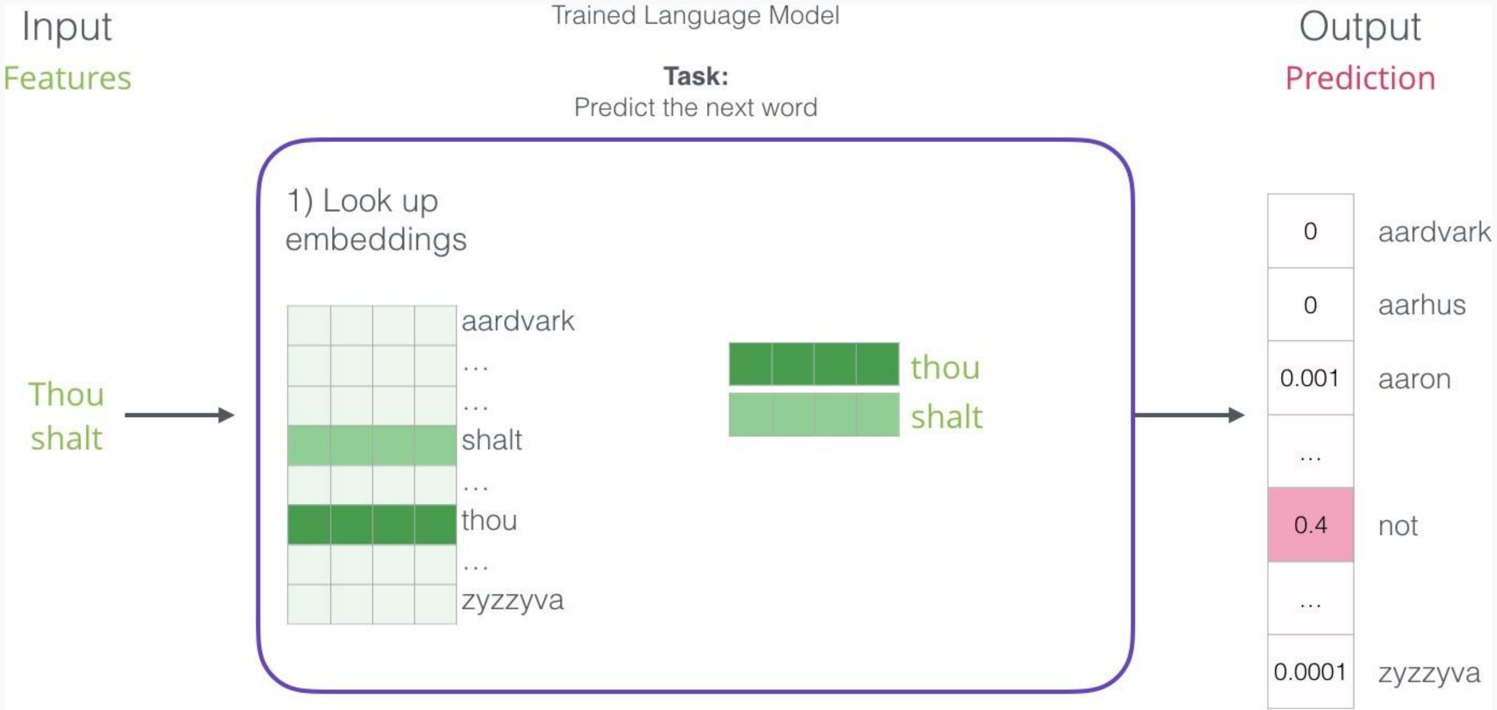
Obligatory example



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	

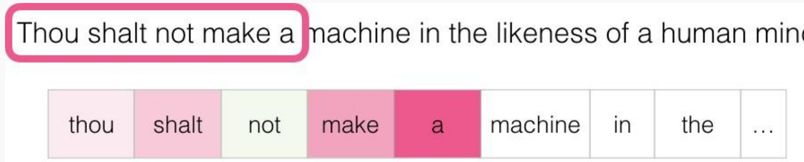
Dataset

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

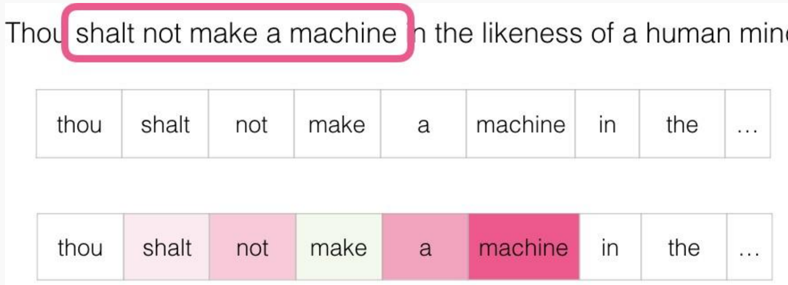
Why not look both ways? This leads to the Skip-Gram and CBOW architectures..

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

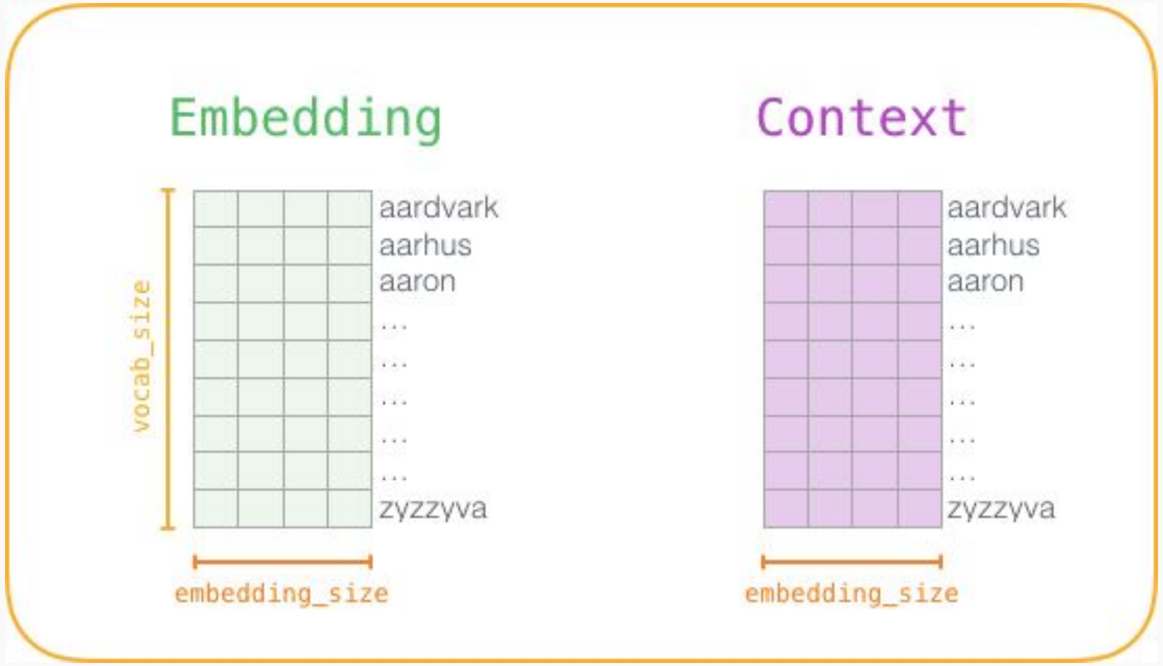


input word	target word
not	thou
not	shalt
not	make
not	a
make	shalt
make	not
make	a
make	machine

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.

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

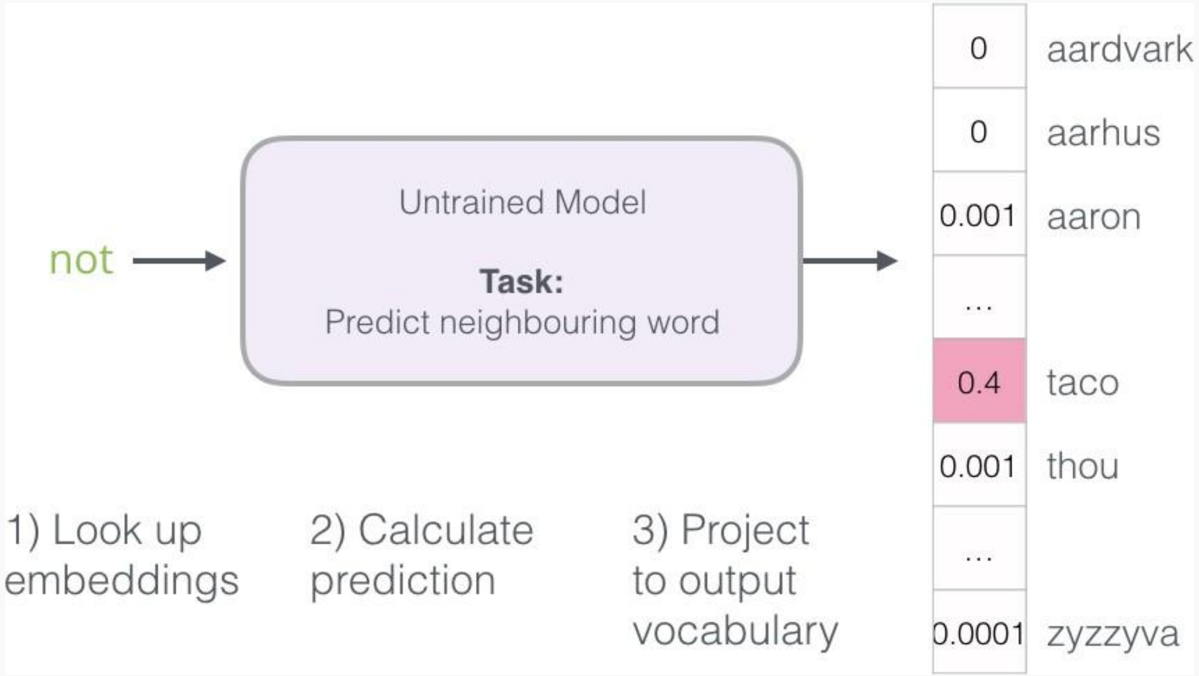
input word	output word	target	input • output
not	thou	1	0.2

Then, assuming a text sequence of length $\boldsymbol{T}$ and window size $\boldsymbol{m}$, 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

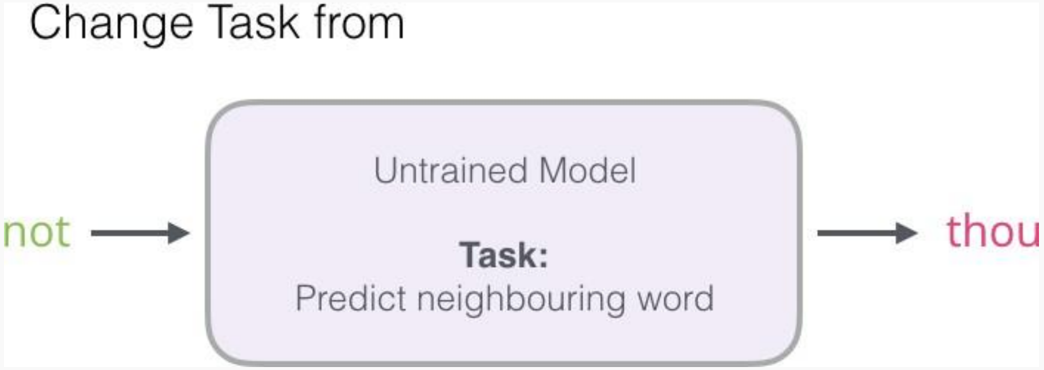
$$\mathbb{P}(w_o \mid w_c) = \frac{\exp(\boldsymbol{u}_o^\top \boldsymbol{v}_c)}{\sum_{i \in \mathcal{V}} \exp(\boldsymbol{u}_i^\top \boldsymbol{v}_c)},$$

- 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:

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

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

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

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

Pick randomly from vocabulary (random sampling)

input word	output word	target
not	thou	1
not	$\boxed{\text{aaron}}$	0
not	$\boxed{\text{taco}}$	0
not	shalt	1
not	make	1

Word	Count	Probability
aardvark		
aarhus		
aaron		
taco		
thou		
zyzzyva		

Likelihood model

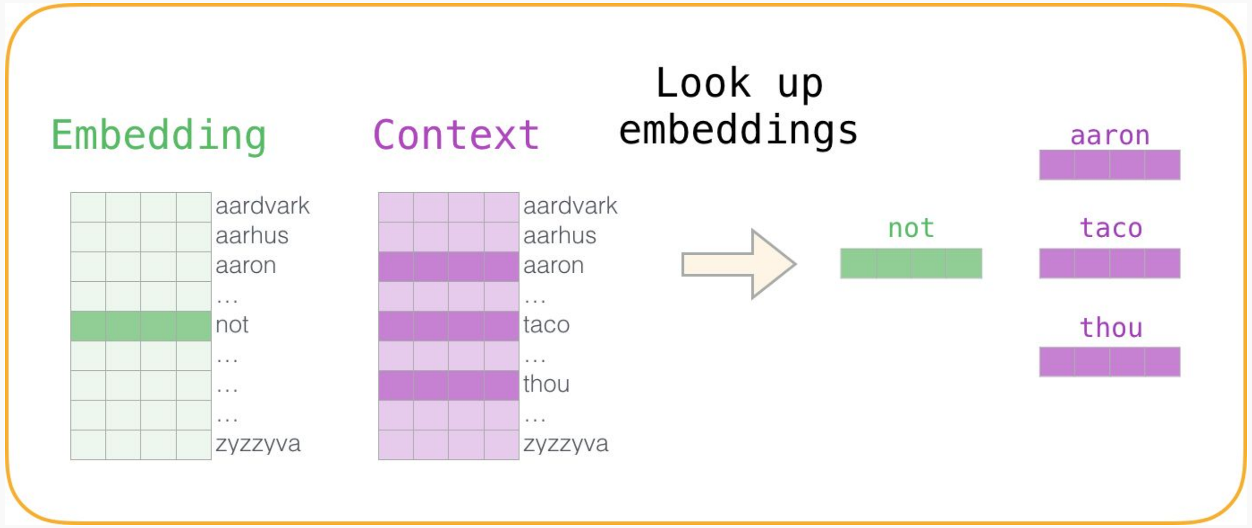
We go back to the old likelihood: $$\mathcal{L} = \prod_{t=1}^{T} \prod_{-m \leq j \leq m,\ j \neq 0} \mathbb{P}(w^{(t+j)} \mid w^{(t)}).$$

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

```python
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
```

```python
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.