Attention in Deep Learning

7. Attention Mechanism and Transformer

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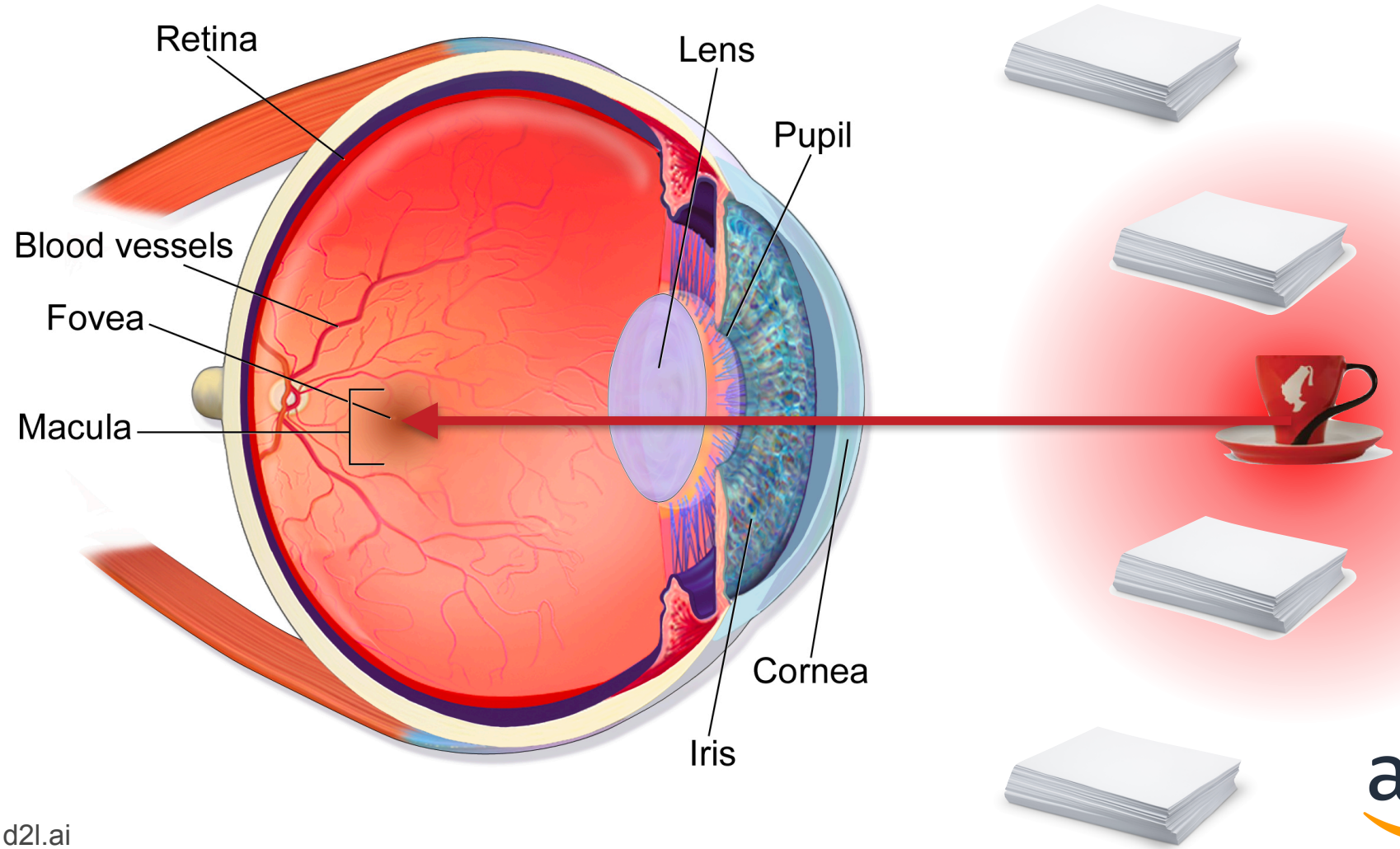
8:30-9:00	Continental Breakfast
9:00-9:45	Introduction and Setup
9:45-10:30	Neural Networks 101
10:30-10:45	Break
10:45-11:15	Machine Learning Basics
11:15-11:45	Context-free Representations for Language
11:45-12:15	Convolutional Neural Networks
12:15-13:15	Lunch Break
13:15-14:00	Recurrent Neural Networks
14:00-14:45	Attention Mechanism and Transformer
14:45-15:00	Coffee Break
15:00-16:15	Contextual Representations for Language
16:15-17:00	Language Generation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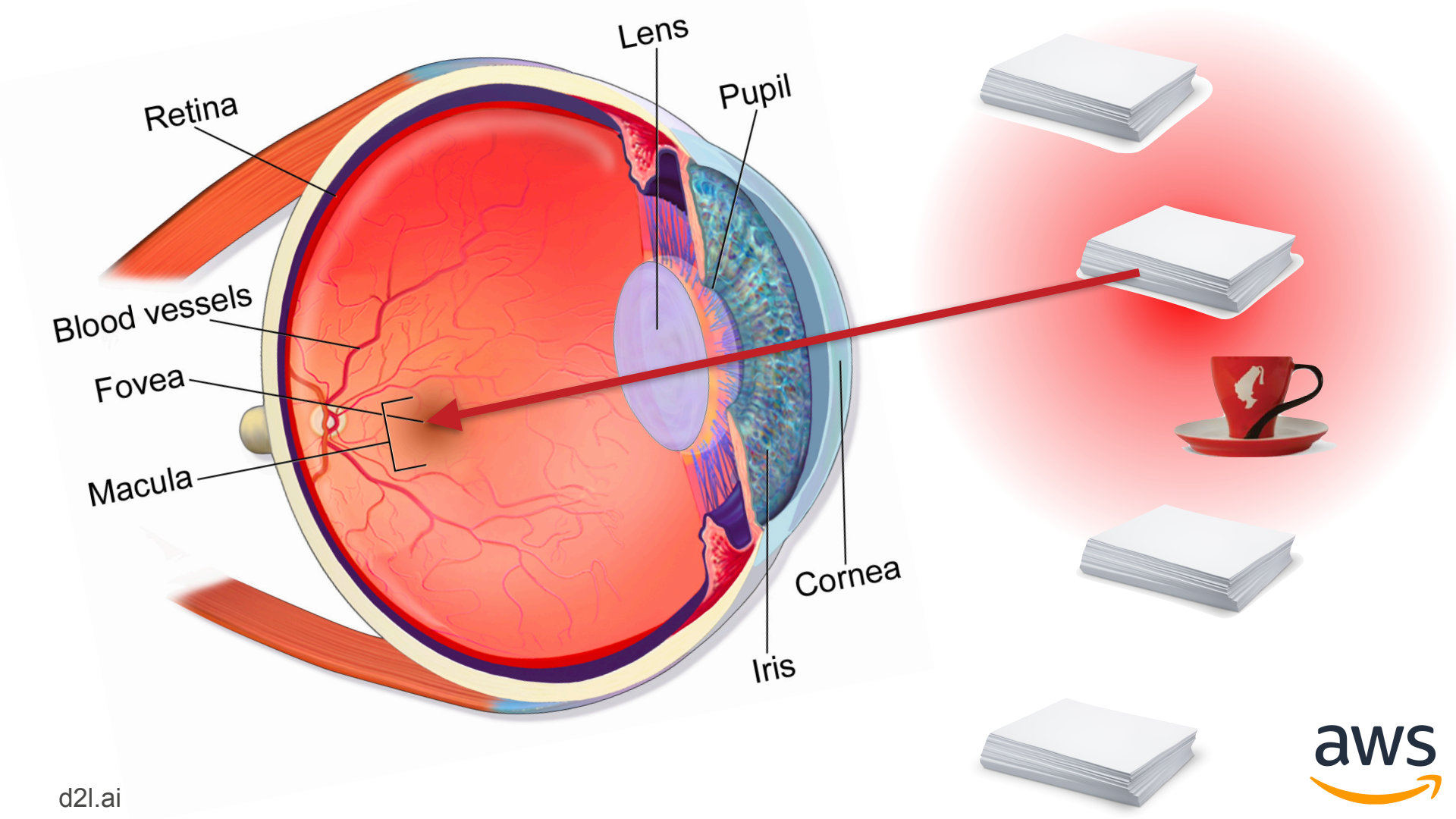
Lens
Pupil
Blood vessels
Fovea
Macula
Cornea
Iris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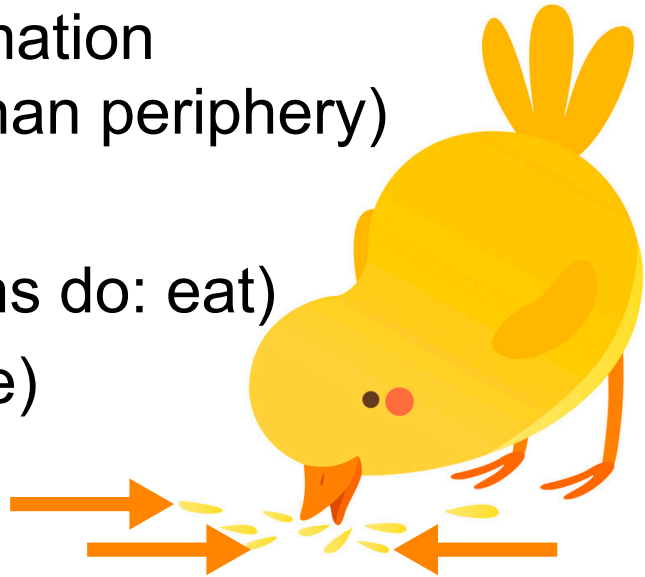
Attention in Animals

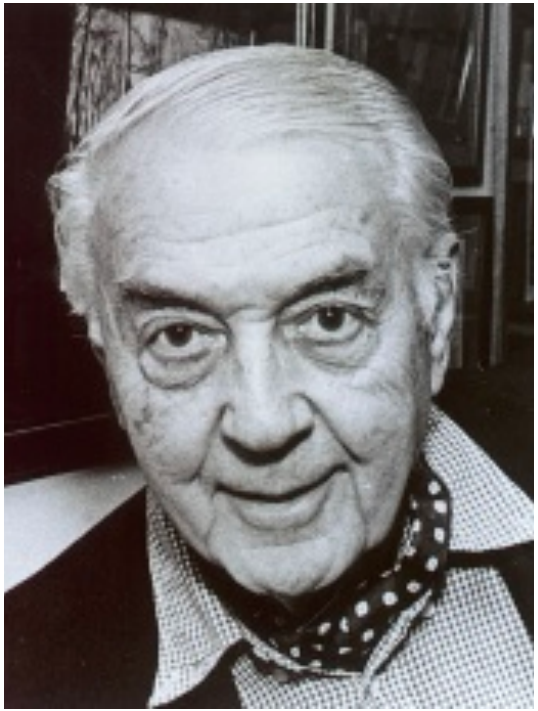
- **Resource saving**
  - Only need **sensors** where relevant bits are (e.g. fovea vs. peripheral vision)
  - Only **compute** relevant bits of information (e.g. fovea has many more ‘pixels’ than periphery)
- **Variable state manipulation**
  - Manipulate environment (for all grains do: eat)
  - Learn modular subroutines (not state)
- **In machine learning - nonparametric**



Outline

1. **Watson Nadaraya Estimator**
2. **Pooling**
   - Single objects - Pooling to attention pooling
   - Hierarchical structures - Hierarchical attention networks
3. **Iterative Pooling and Generation**
   Neural machine translation
4. **Multiple Attention Heads**
   - Transformers / BERT
   - Lightweight, structured, sparse
5. **Resources**

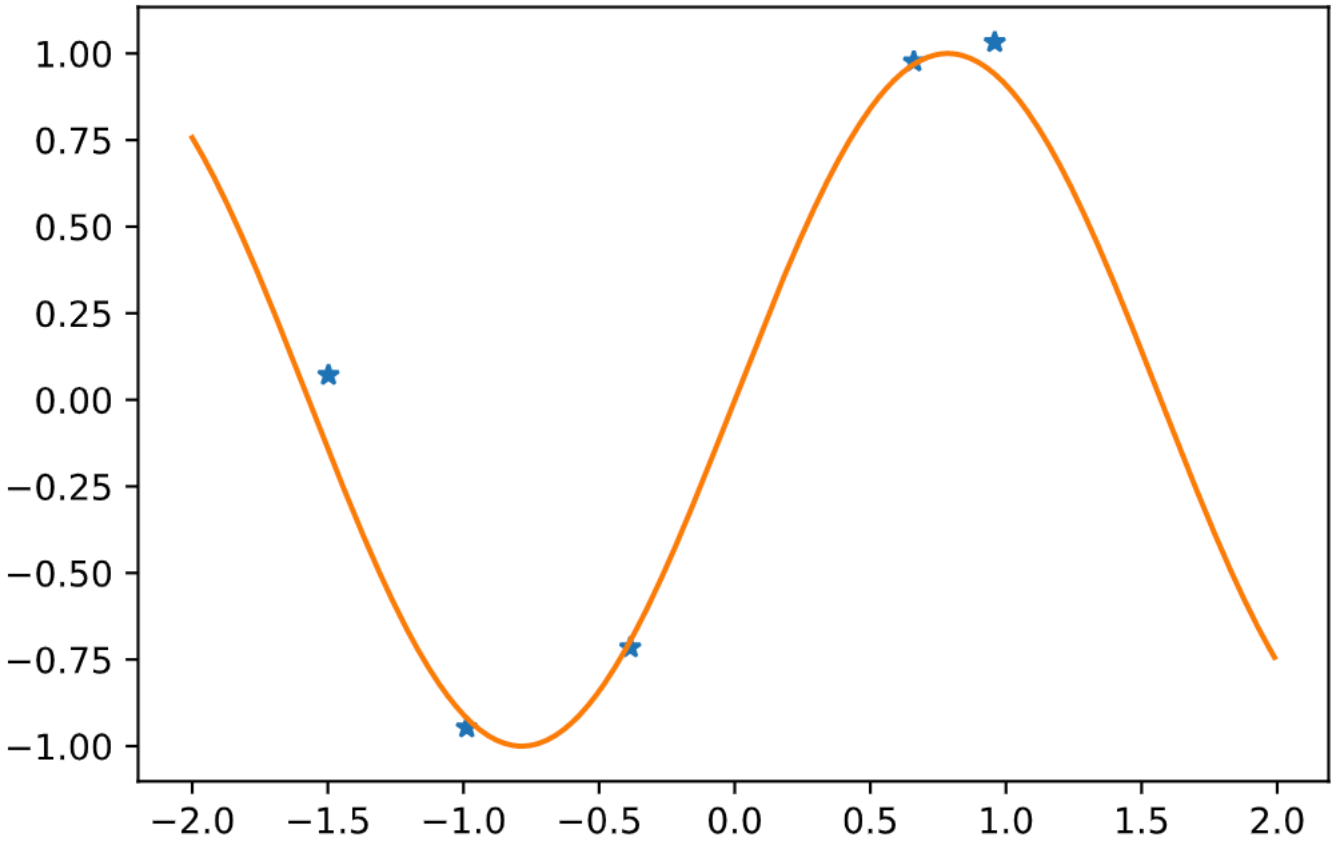
1. Watson Nadaraya Estimator ‘64



Geoffrey Watson

Elizbar Nadaraya

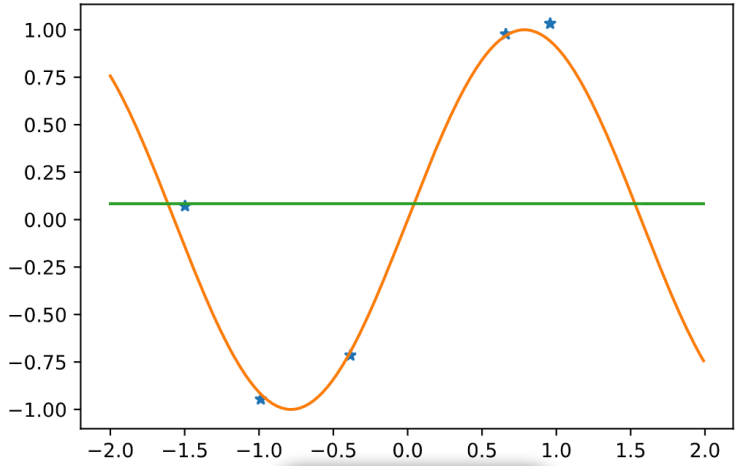
Regression Problem



Solving the regression problem

- Data $\{x_1, \ldots x_m\}$ and labels $\{y_1, \ldots y_m\}$
- Estimate label y at new location x
- **The world's dumbest estimator**
  Average over all labels

$$y = \frac{1}{m} \sum_{i=1}^{m} y_i$$



- **Better idea (Watson, Nadaraya, 1964)**
  Weigh the labels according to location

$$y = \sum_{i=1}^{m} \alpha(x, x_i) y_i$$

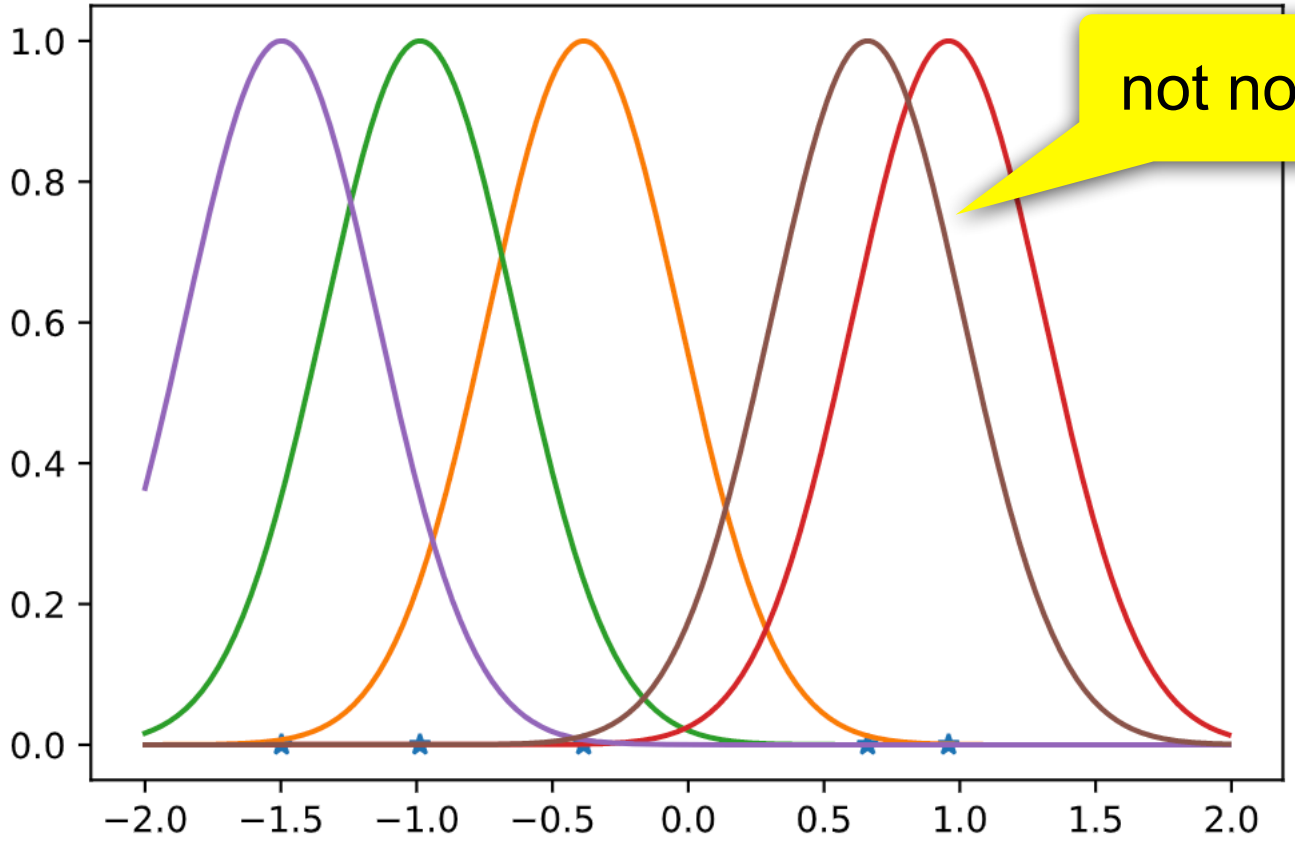
key

$\alpha(x, x_i) y_i$

query

value

Weighing the locations (e.g. with Gaussians)



not normalized

$$\alpha(x, x_i) \propto k(x_i, x)$$

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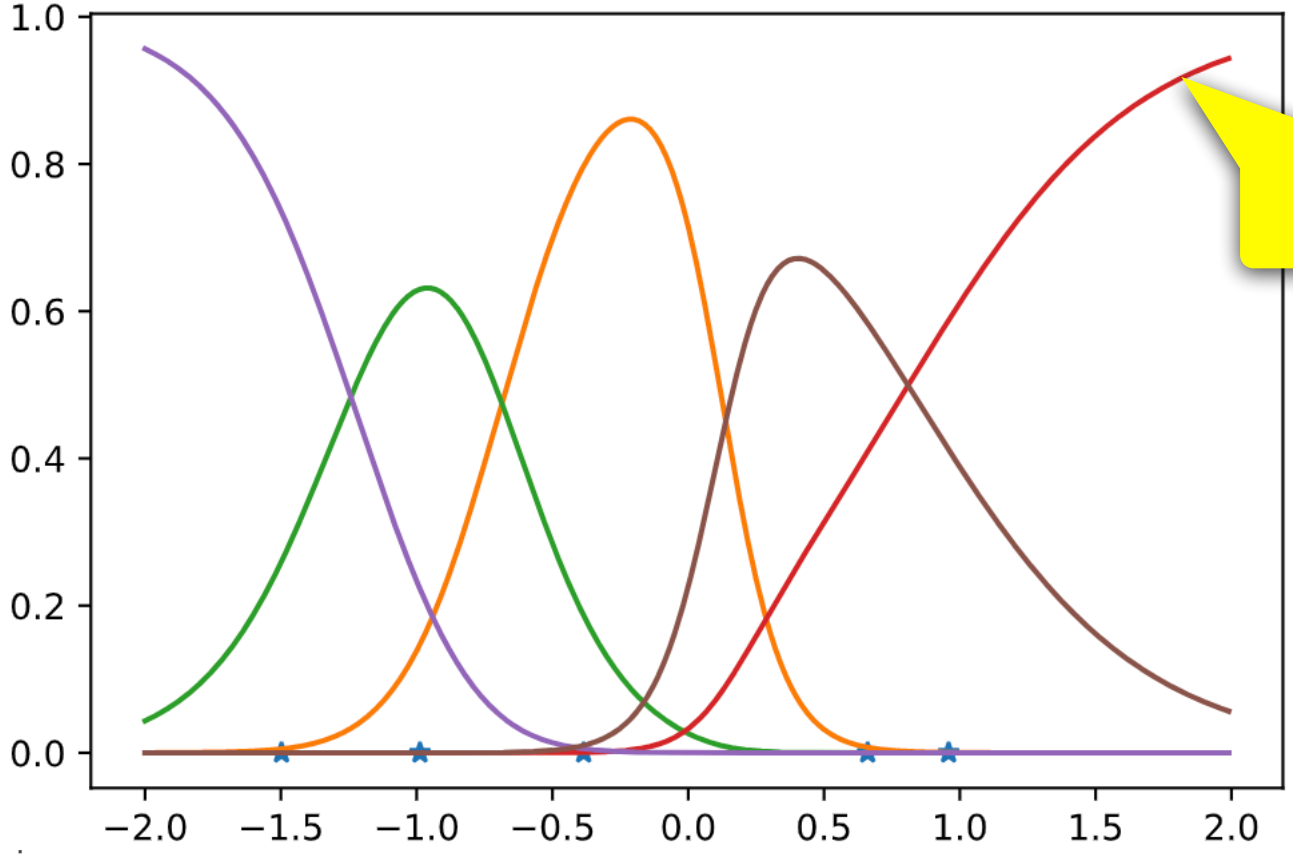
Weighing the locations (e.g. with Gaussians)



normalized

$$\alpha_i(x) = \frac{k(x_i, x)}{\sum_j k(x_j, x)}$$

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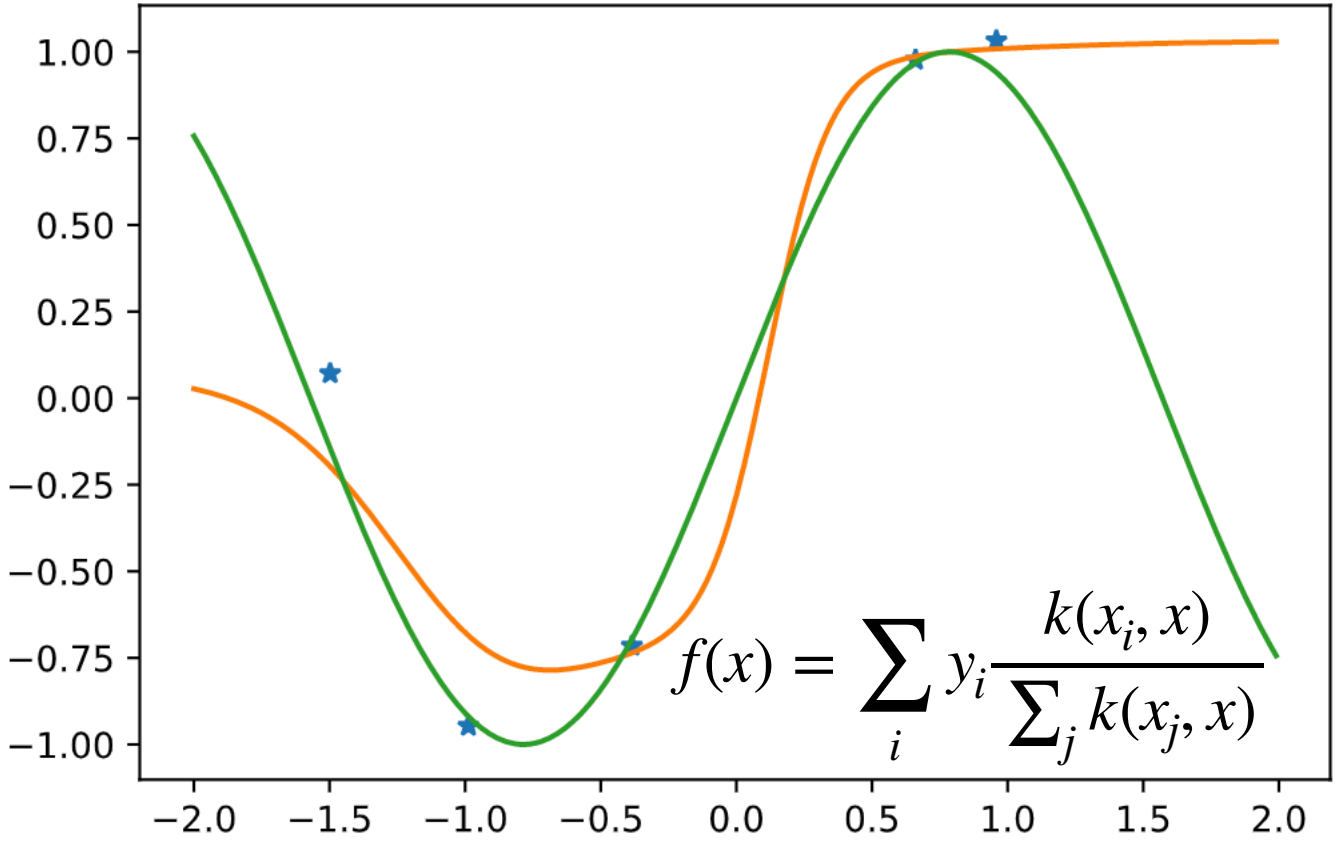
Weighted regression estimate



Why bother with a 55 year old algorithm?

- **Consistency**
  Given enough data this algorithm converges to the optimal solution (can your deep net do this?)
- **Simplicity**
  No free parameters - information is in the data not weights (or very few if we try to learn the weighting function)


2. Pooling

Deep Sets (Zaheer et al. 2017)

- Deep (Networks on) Sets $X = \{x_1, \ldots x_n\}$
  - Need permutation invariance for elements in set (e.g. LSTM doesn't work to ingest elements)
  - Theorem - all functions are of the form*

$$f(X) = \rho\left(\sum_{x \in X} \phi(x)\right)$$

*or some combination thereof

- Applications - point clouds, set extension, red shift for galaxies, text retrieval, tagging, etc.

Deep Sets (Zaheer et al. 2017)

Outliers in sets - learn function $f(X)$ on set such that

$$f(\{x\} \cup X) \geq f\left(\{x'\} \cup X\right) + \Delta\left(x, x'\right)$$

Deep Sets with Attention aka Multi-Instance Learning (Ilse, Tomczak, Welling, '18)

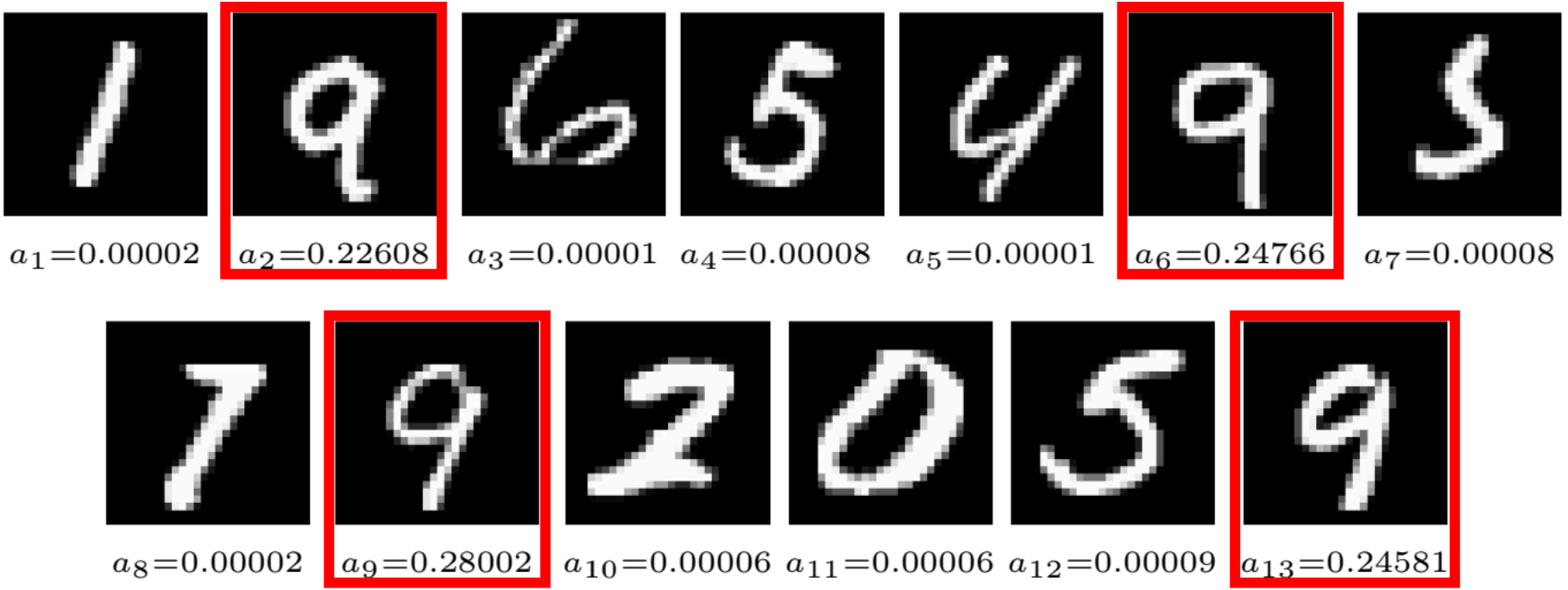
- Multiple Instance Problem
  Set contains one (or more) elements with desirable property (drug discovery, keychain). Identify those sets.
- Deep Sets have trouble focusing, hence weigh it

$$f(X) = \rho\left(\sum_{x \in X} \phi(x)\right) \longrightarrow f(X) = \rho\left(\sum_{x \in X} \alpha(w, x)\phi(x)\right)$$

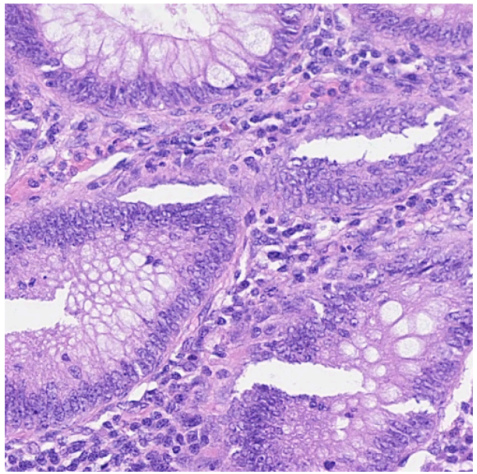
- Attention function e.g. $\alpha(w, x) \propto \exp\left(w^\top \tanh Vx\right)$

Deep Sets with Attention aka Multi-Instance Learning (Ilse, Tomczak, Welling, ’18)

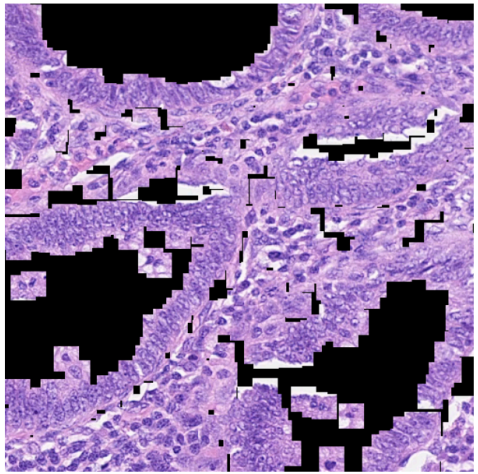
Identifying sets that contain the digit ‘9’



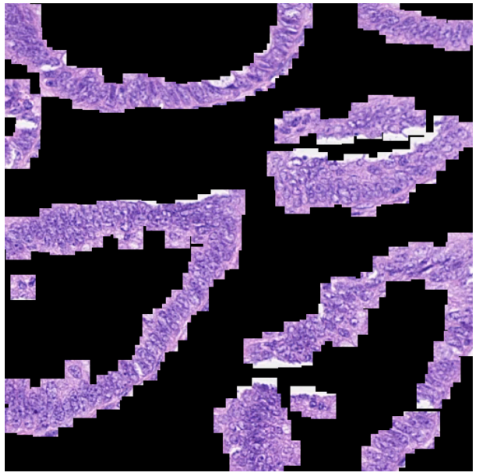
Deep Sets with Attention aka Multi-Instance Learning (Ilse, Tomczak, Welling, ’18)



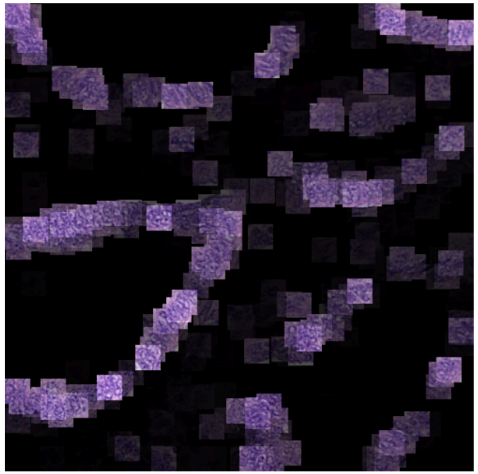
tissue sample



windowed cell nuclei



cancerous cells



attention weights

Bag of words (Salton & McGill, 1986)
Word2Vec (Mikolov et al., 2013)

- Embed each word in sentence (word2vec, binary, GRU …)
- Add them all up
- Classify

$$f(X) = \rho\left(\sum_{i=1}^{n} \phi(x_i)\right)$$

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The tutorial is awesome.
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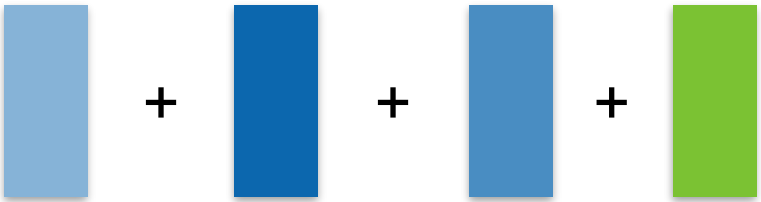
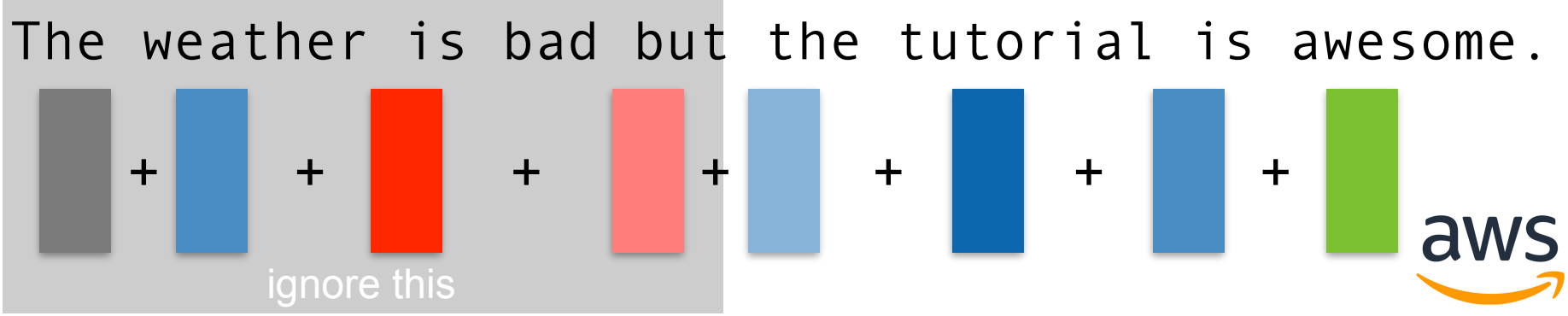


Bag of words (Salton & McGill, 1986)
Word2Vec (Mikolov et al., 2013)

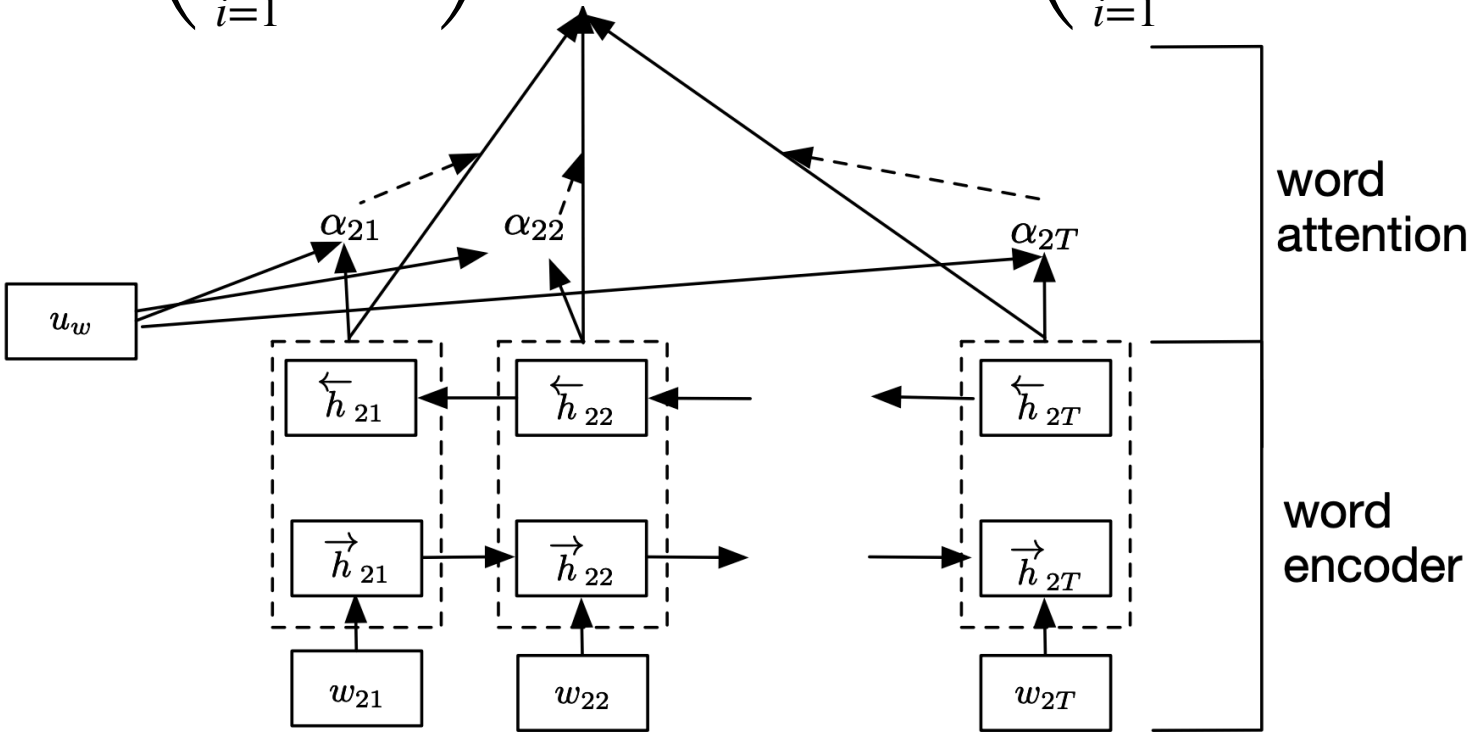
- Embed each word in sentence (word2vec, binary, GRU …)
- Add them all up
- Classify

$$f(X) = \rho\left(\sum_{i=1}^{n} \phi(w_i)\right)$$



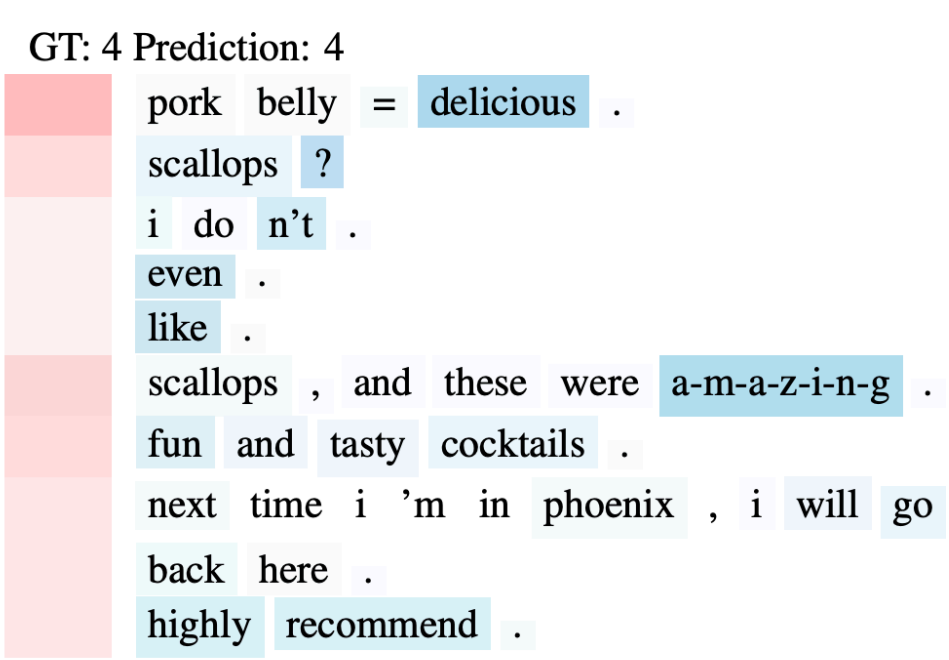
Attention weighting for documents (Wang et al, ’16)

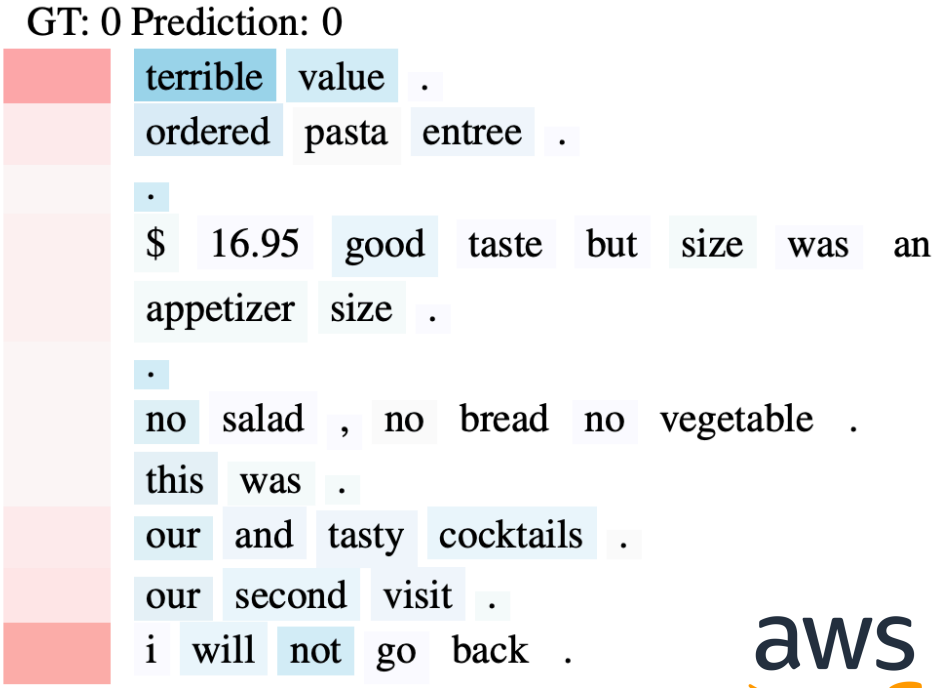
$$f(X) = \rho\left(\sum_{i=1}^{n} \phi(w_i)\right) \rightarrow f(X) = \rho\left(\sum_{i=1}^{n} \alpha(w_i, X)\phi(w_i)\right)$$



Hierarchical attention weighting (Yang et al. ’17)

Some sentences are more important than others …





Hierarchical attention

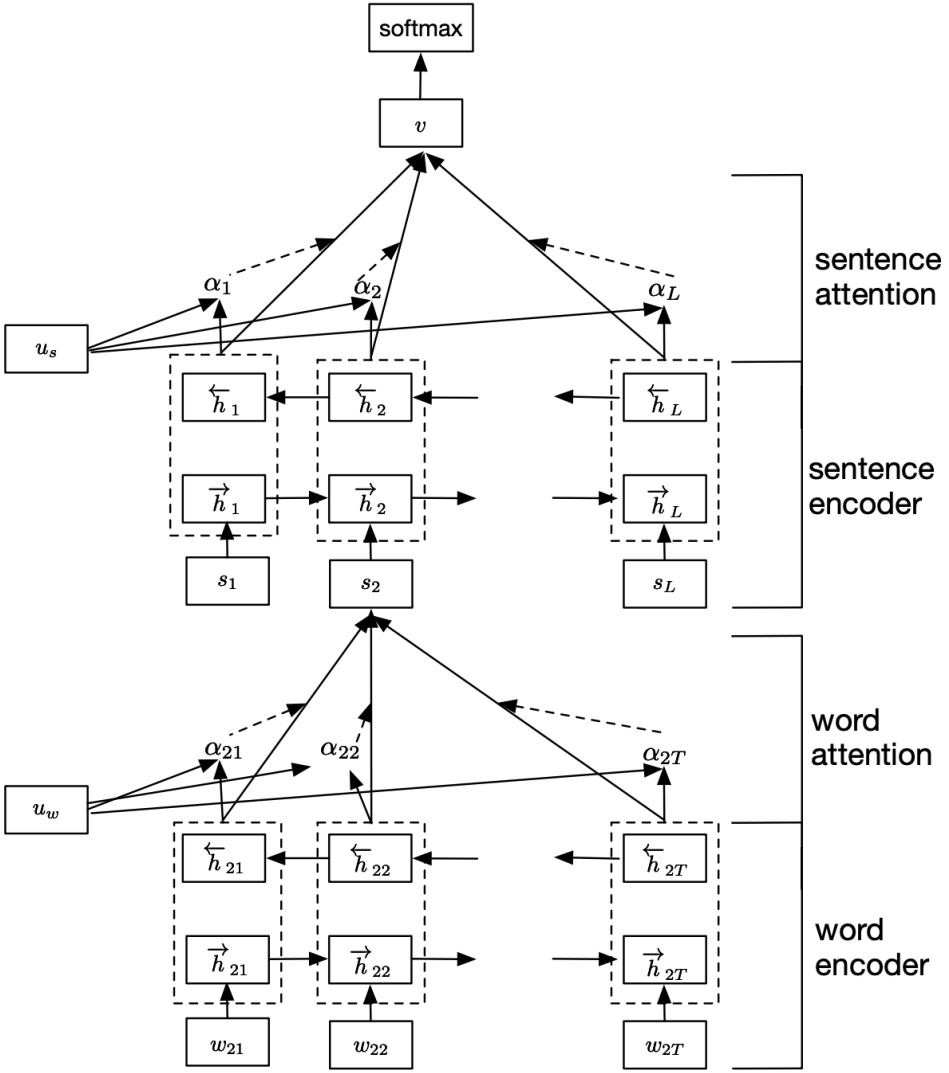
- Word level

$$f(s_i) = \rho\left(\sum_{j=1}^{n_i} \alpha(w_{ij}, s_i)\phi(w_{ij})\right)$$

- Sentence level

$$g(d) = \rho\left(\sum_{i=1}^{n} \alpha(s_i, d)\phi(f(s_i))\right)$$

- Embeddings e.g. via GRU



Attention Summary

- Pooling

$$f(X) = \rho\left(\sum_{x \in X} \phi(x)\right)$$

- Attention pooling

$$f(X) = \rho\left(\sum_{x \in X} \alpha(x, w)\phi(x)\right)$$

Query w can depend on context

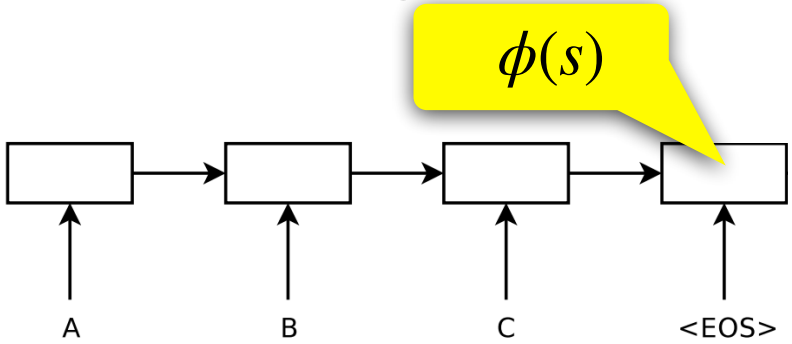
- Attention function (normalized to unit weight) such as

$$\alpha(x, X) \propto \exp\left(w^\top \tanh Ux\right)$$


3. Iterative
Output

Seq2Seq for Machine Translation, Sutskever, Vinyals, Le '14

- Encode source sequence s via LSTM to representation $\phi(s)$
- Decode to target sequence one character at a time

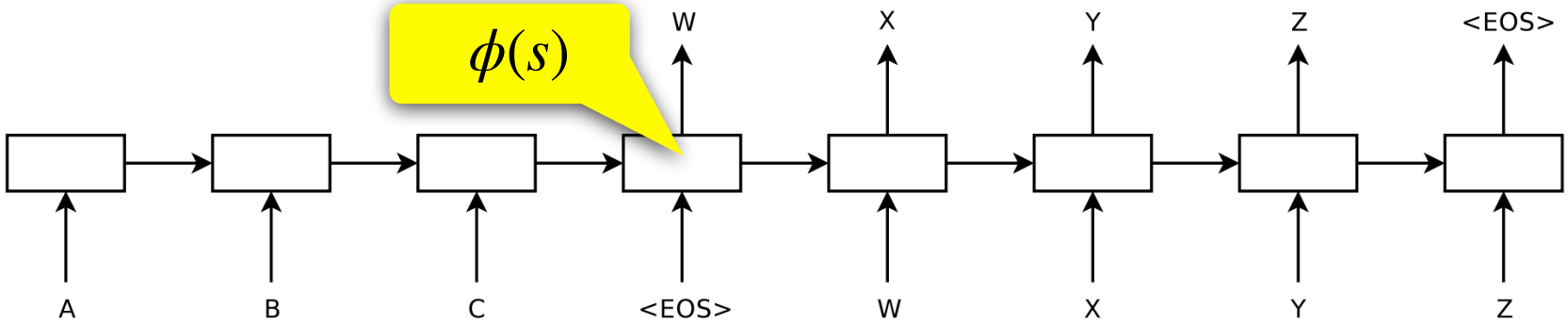


- 'The table is round.' - 'Der Tisch ist rund.'
- 'The table is very beautiful with r , blah blah blah blah' - 'Error …'

Representation not rich enough

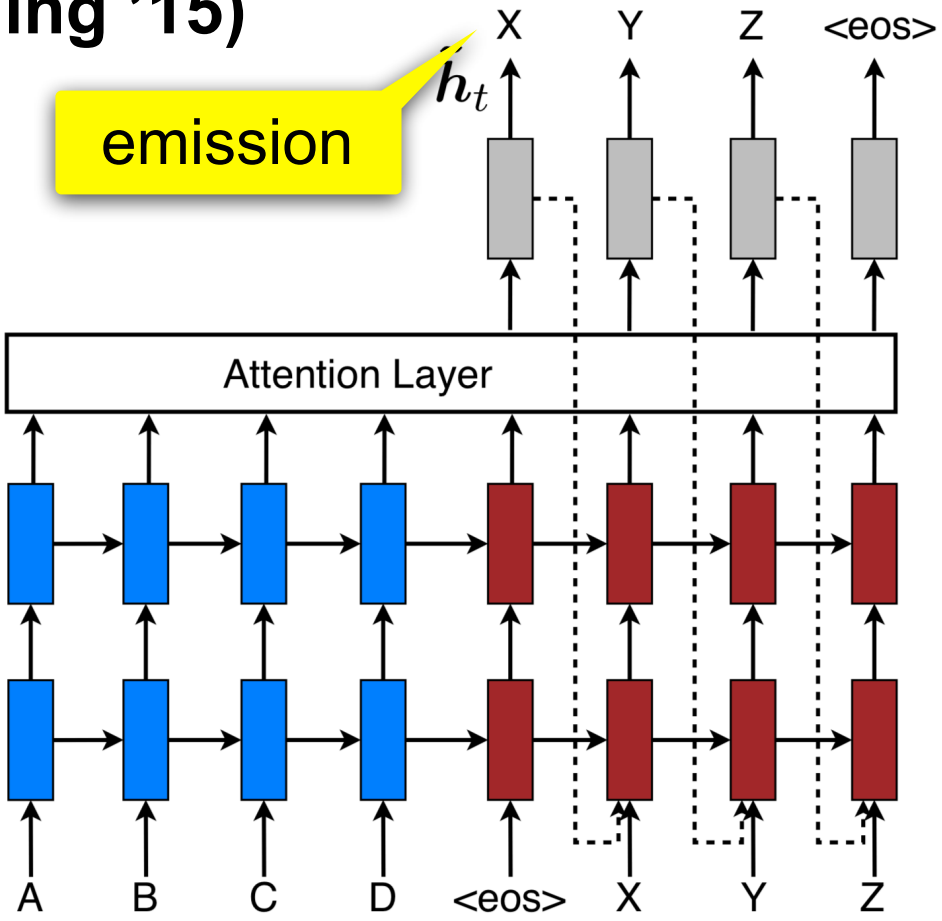
Seq2Seq for Machine Translation, Sutskever, Vinyals, Le '14

- Encode source sequence s via LSTM to latent representation $\phi(s)$
- Decode to target sequence one character at a time



- Need memory for long sequences
- Attention to iterate over source
  (we can look up source at any time after all)

Seq2Seq with attention (Bahdanau, Cho, Bengio '14) (Pham, Luong, Manning '15)



Seq2Seq with attention (Bahdanau, Cho, Bengio '14) (Pham, Luong, Manning '15)

$$\alpha_{ij} \propto \exp(a(\tilde{h}_{i-1}, h_j))$$

query

key & value

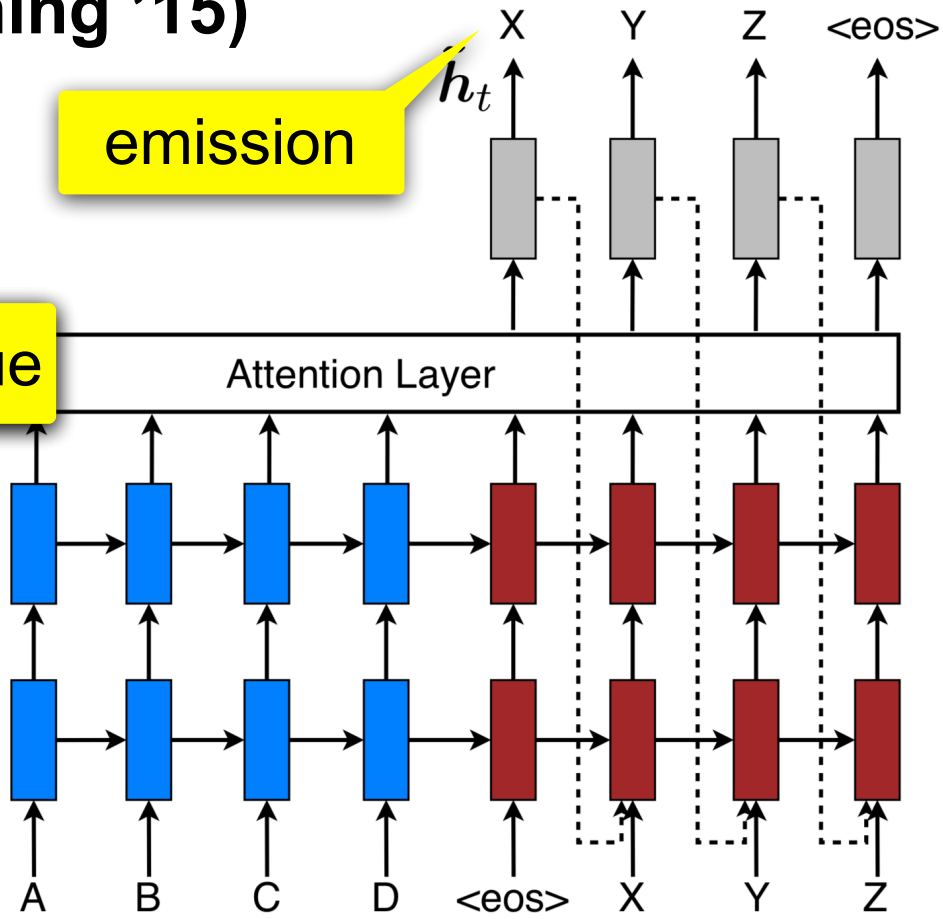
$$c_i = \sum_{j=1}^{n} \alpha_{ij} h_j$$

$$\tilde{h}_i = f(s_{i-1}, y_{i-1}, c_i)$$

y_i

emission

h_t



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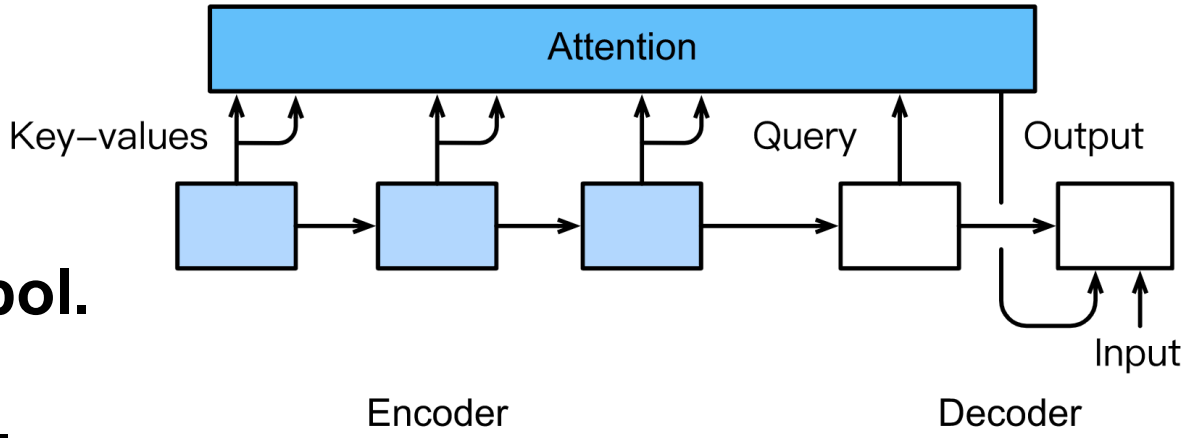
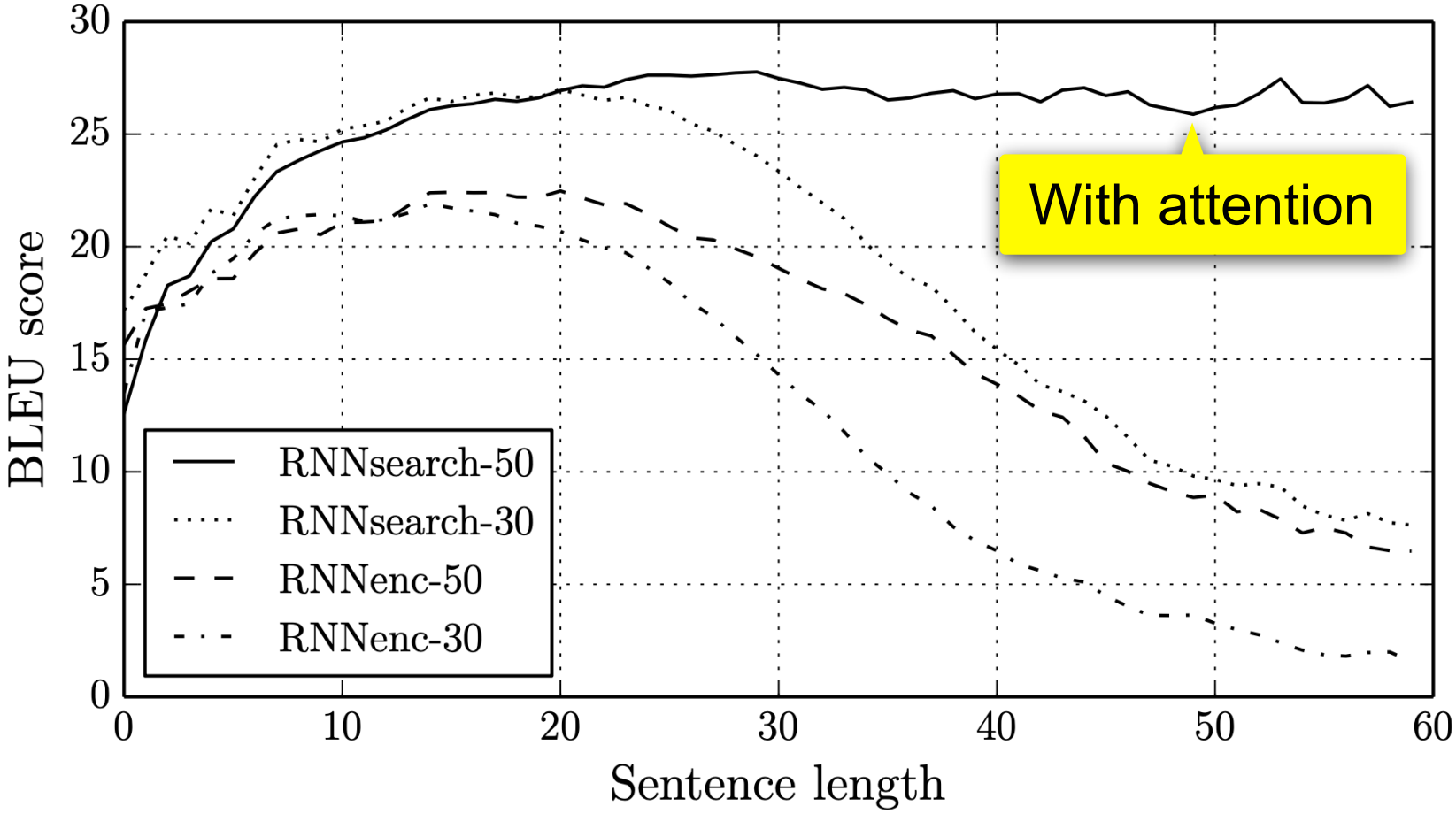
Seq2Seq with attention (Bahdanau, Cho, Bengio '14) (Pham, Luong, Manning '15)

- Iterative attention model
  - Compute (next) attention weights
  - Aggregate next state
  - Emit next symbol
- Repeat
- **Memory networks emit only one symbol.**
- **NMT with attention emits many symbols.**



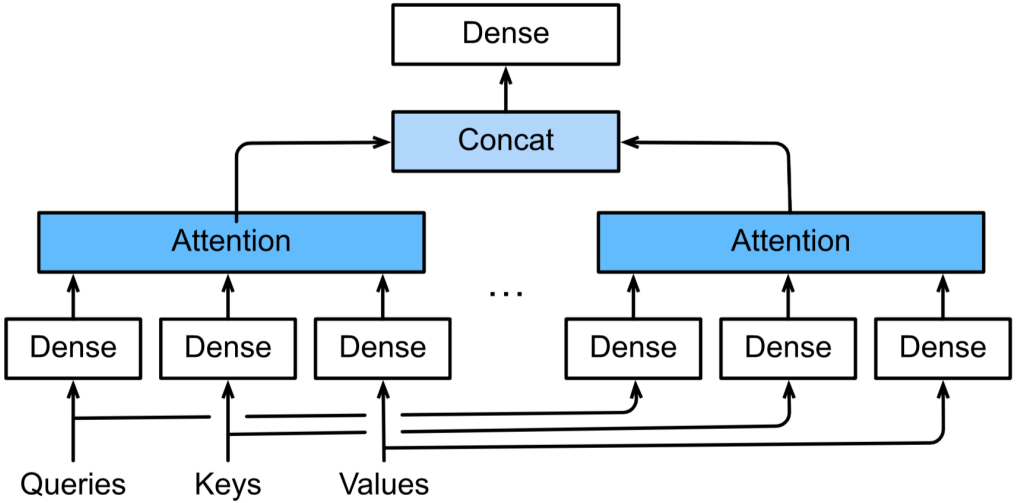
Seq2Seq with attention (Bahdanau, Cho, Bengio '14)



5. Multiple Heads

Multi-head attention (Vaswani et al., '17)

Q: query
K: key
V: value



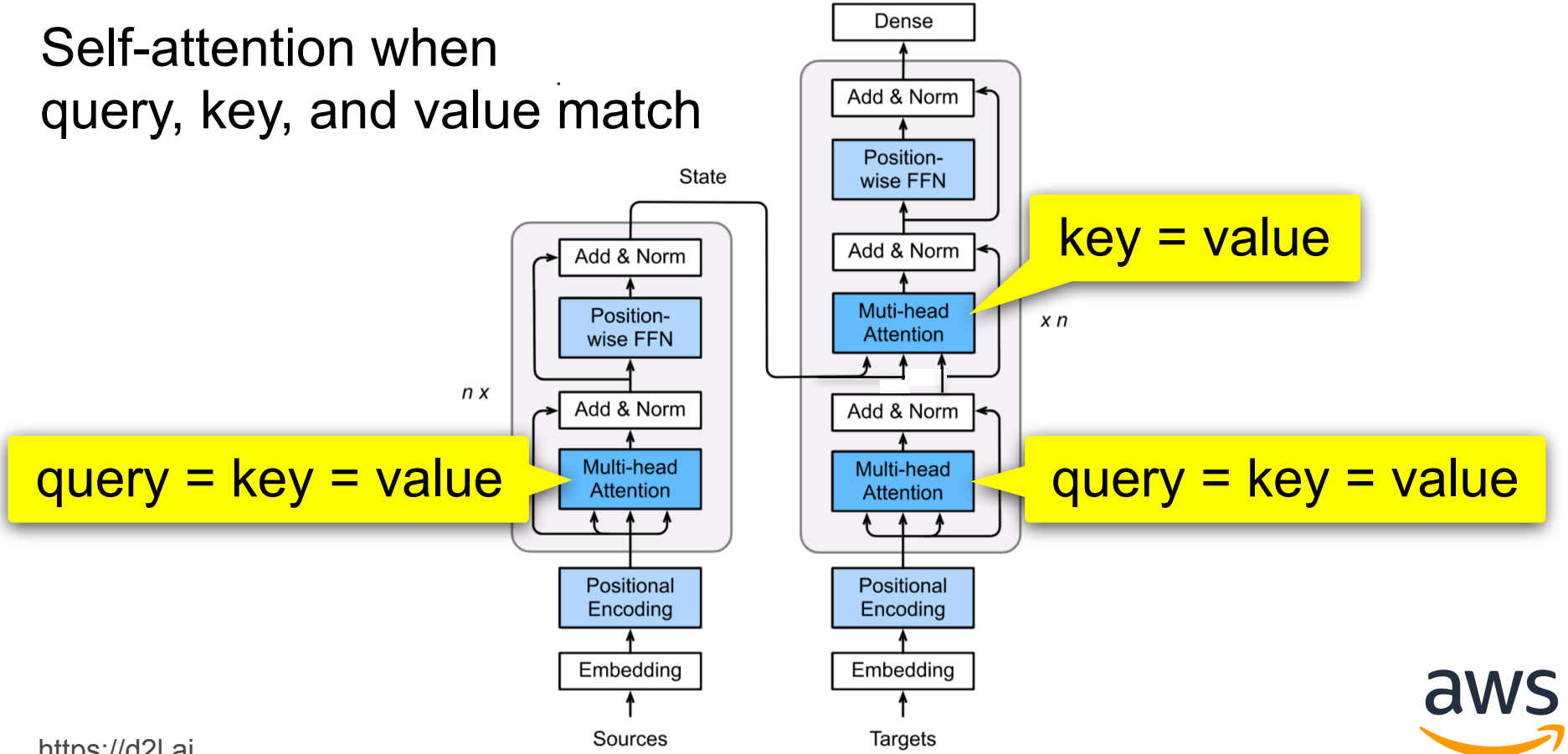
$$\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)V$$

$$\text{MultiHead}(Q, K, V) = \text{Concat}(\text{head}_1, \ldots \text{head}_h)W^O$$

$$\text{where head}_i = \text{Attention}\left(QW_i^Q, KW_i^K, VW_i^V\right)$$

Transformer with multi-head attention (Vaswani et al., ‘17)

Self-attention when
query, key, and value match



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