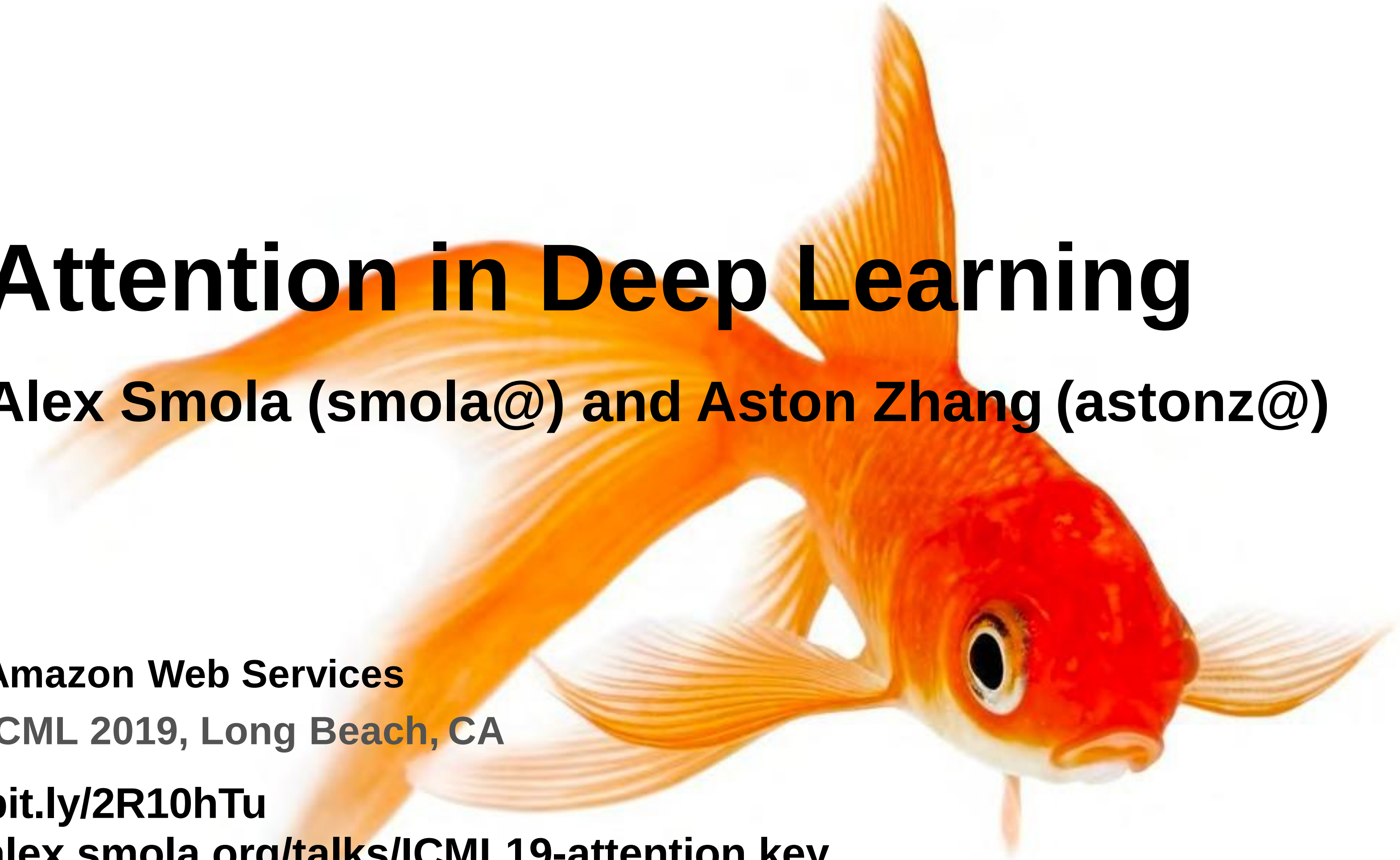


Attention in Deep Learning

Alex Smola (smola@) and Aston Zhang (astonz@)

Amazon Web Services

ICML 2019, Long Beach, CA

bit.ly/2R10hTu
alex.smola.org/talks/ICML19-attention.key
alex.smola.org/talks/ICML19-attention.pdf

Outline

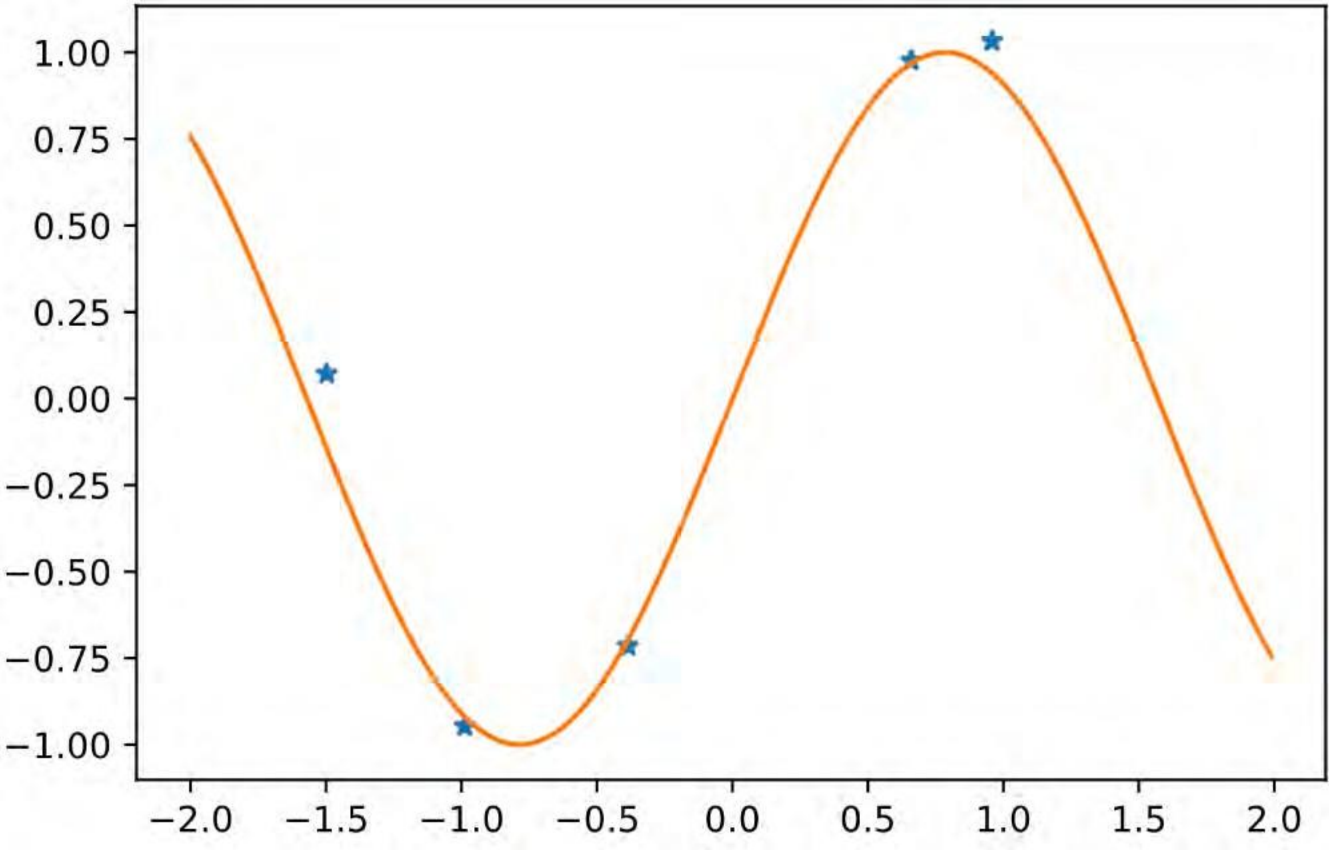
1. **Watson Nadaraya Estimator**
2. **Pooling**
    - Single objects - Pooling to attention pooling
    - Hierarchical structures - Hierarchical attention networks
3. **Iterative Pooling**
   Question answering / memory networks
4. **Iterative Pooling and Generation**
   Neural machine translation
5.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

1. Watson Nadaraya Estimator ‘64

Geoffrey Watson

Elizbar Nadaraya

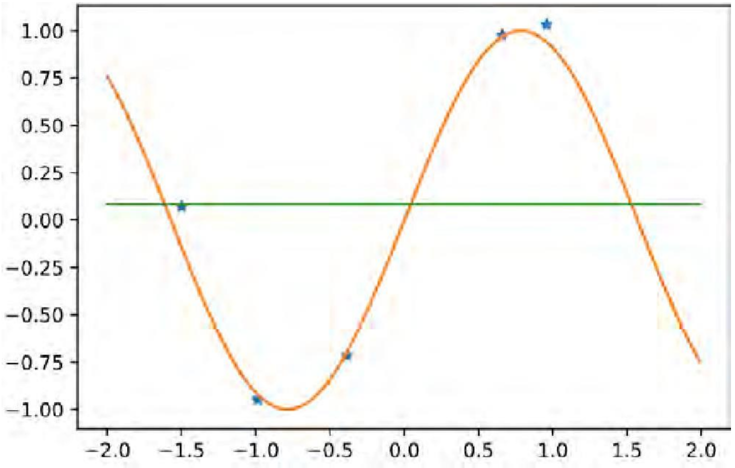
Regression Problem



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

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

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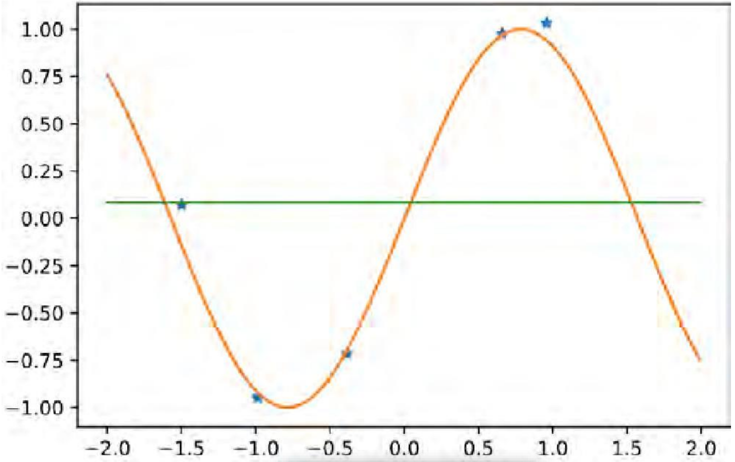


- **Better idea (Watson, Nadaraya, 1964)**
  Weigh the labels according to **location**

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

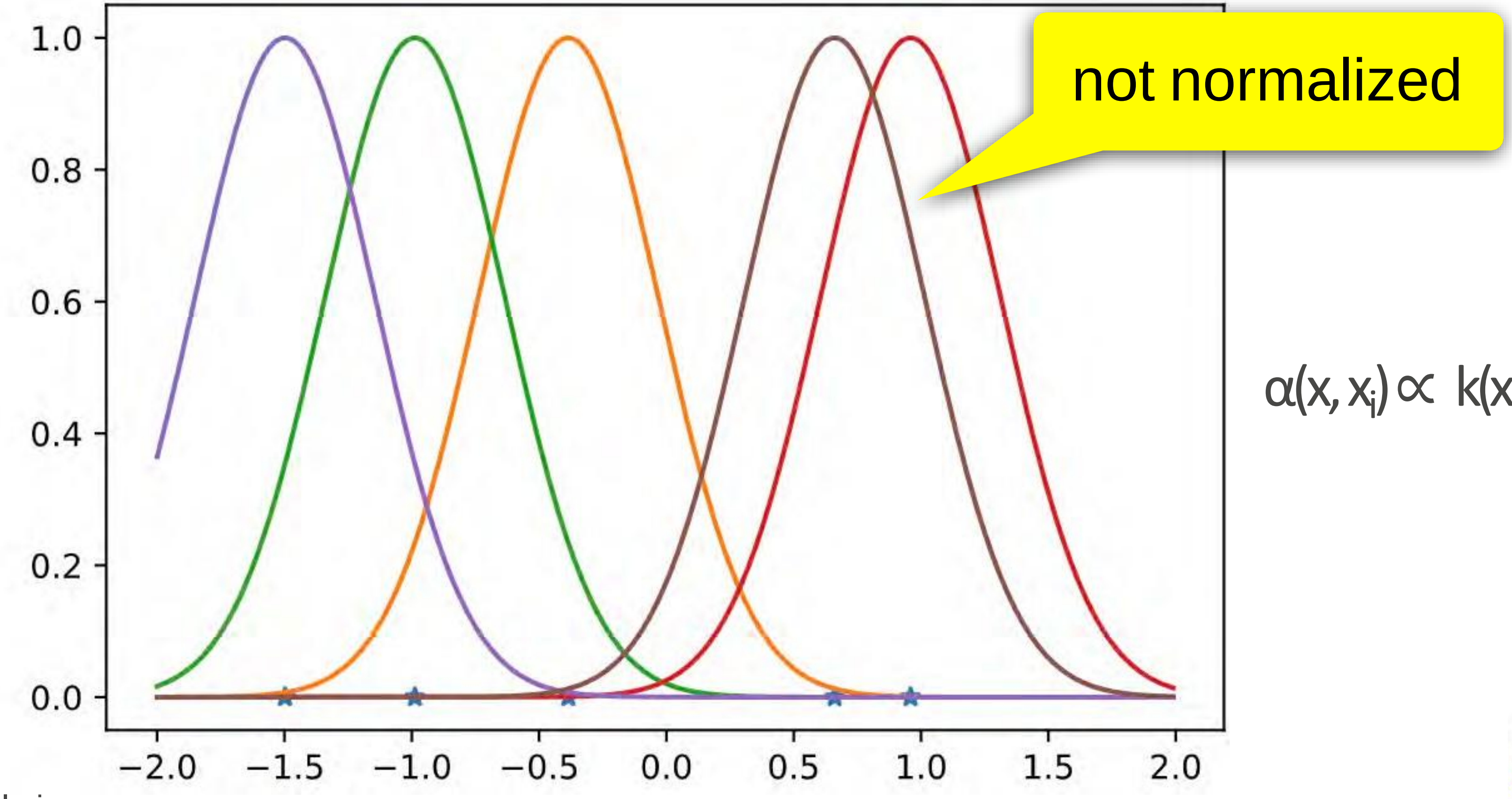
key

$\alpha(x,x_i)y_i$

query

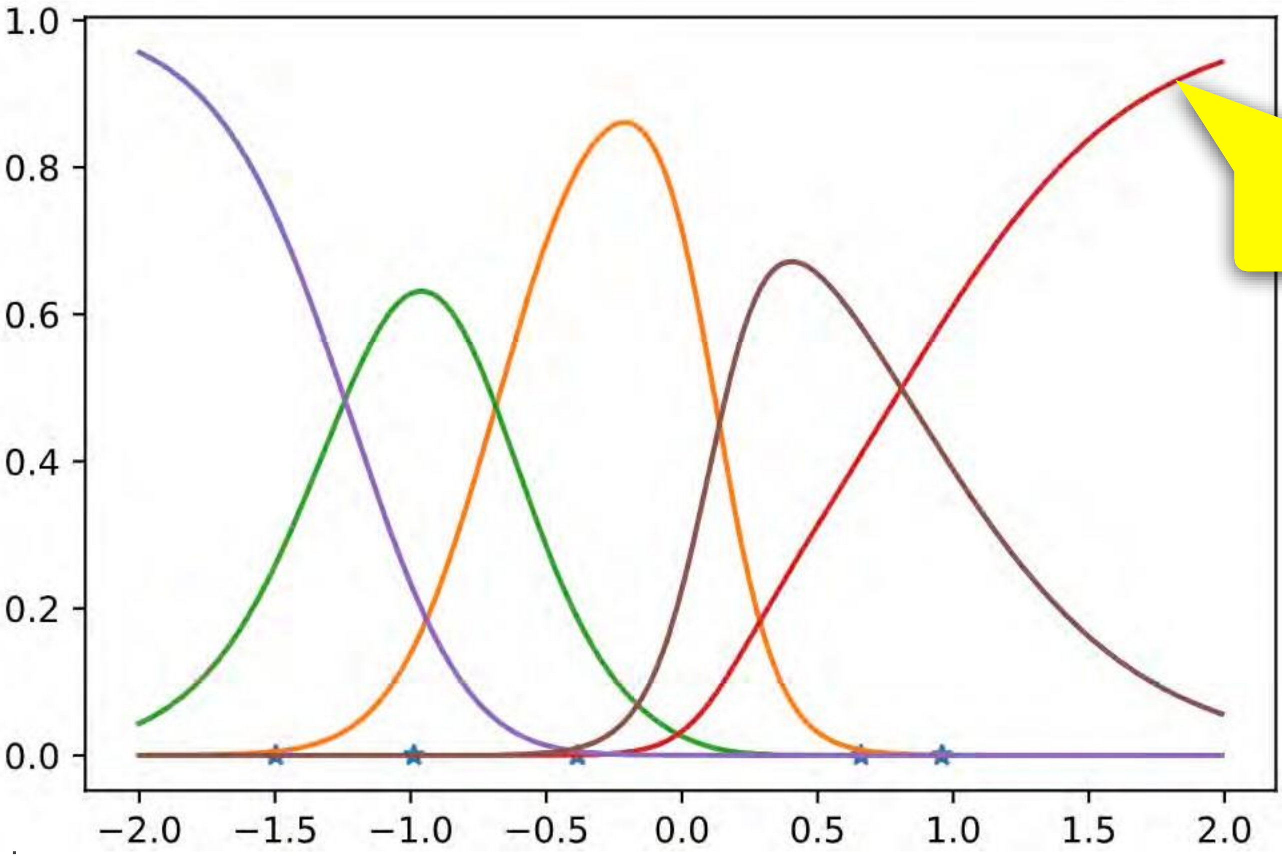
value

Weighing the locations (e.g. with Gaussians)



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

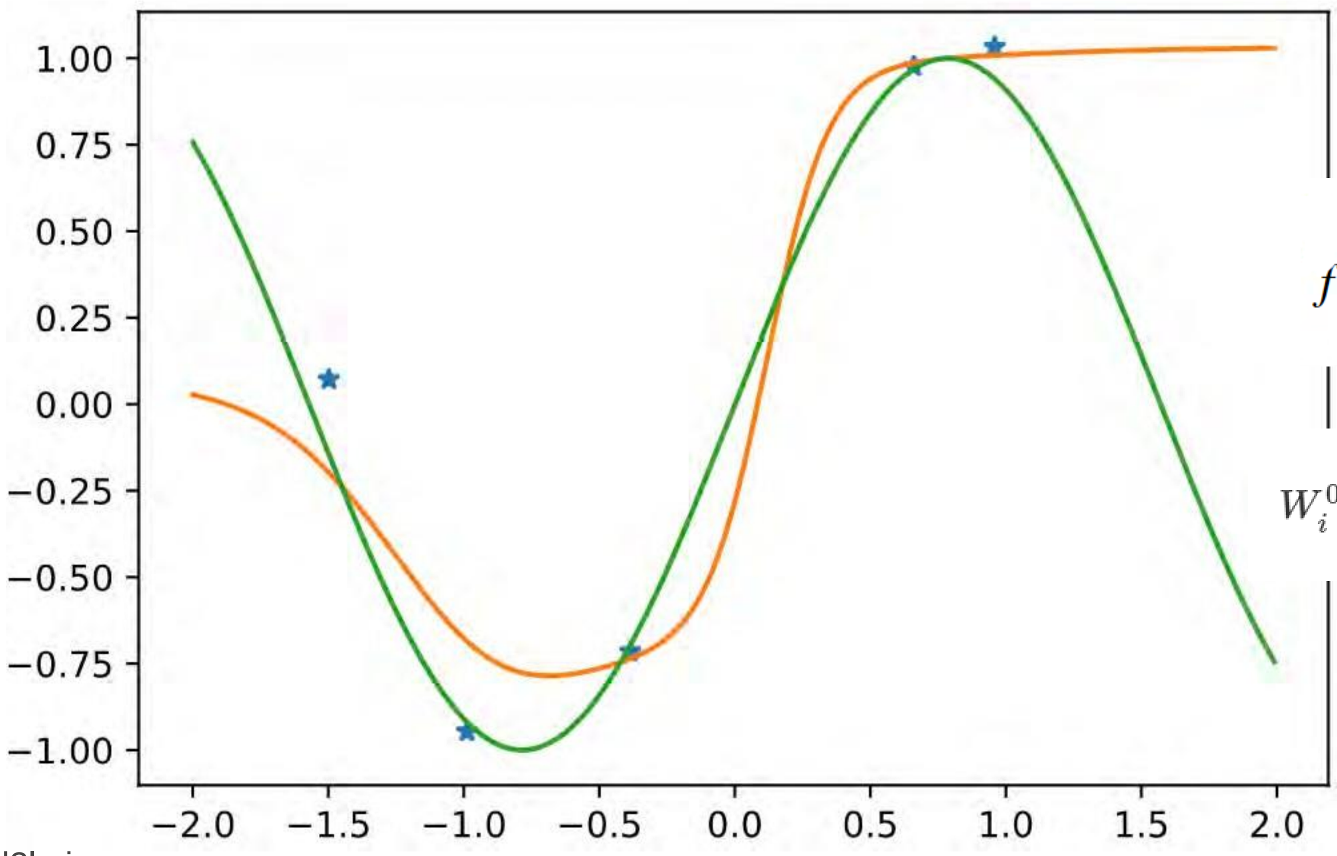
Weighing the locations (e.g. with Gaussians)



normalized

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

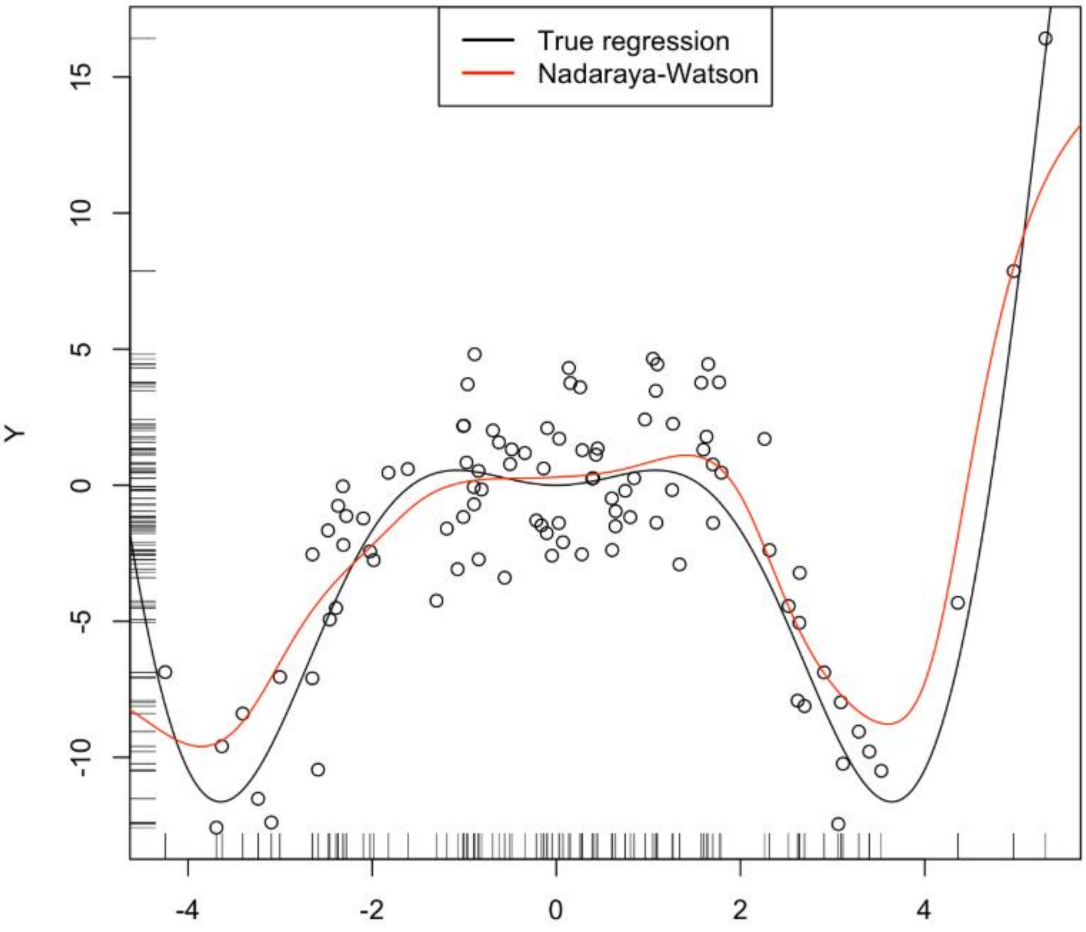
Weighted regression estimate



Wi(x)

$$f(x) = \sum_i y_i \boxed{\frac{k(x_i, x)}{\sum_j k(x_j, x)}}$$

$$W_i^0(x) := \frac{K_h(x - X_i)}{\sum_{i=1}^{n} K_h(x - X_i)}.$$


True regression
Nadaraya-Watson
Y
15
10
5
0
-5
-10
-4
-2
0
2
4

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)

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- **Deep Learning Variant**
  - Learn weighting function
  - Replace averaging (pooling) by weighted pooling

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

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

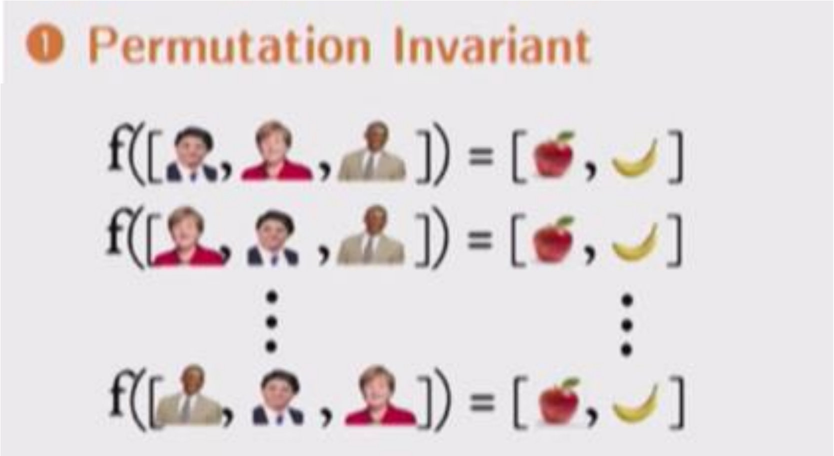
Deep Sets with Attention aka Multi-Instance Learning (Ilse, Tomczak, Welling, '18)

- 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

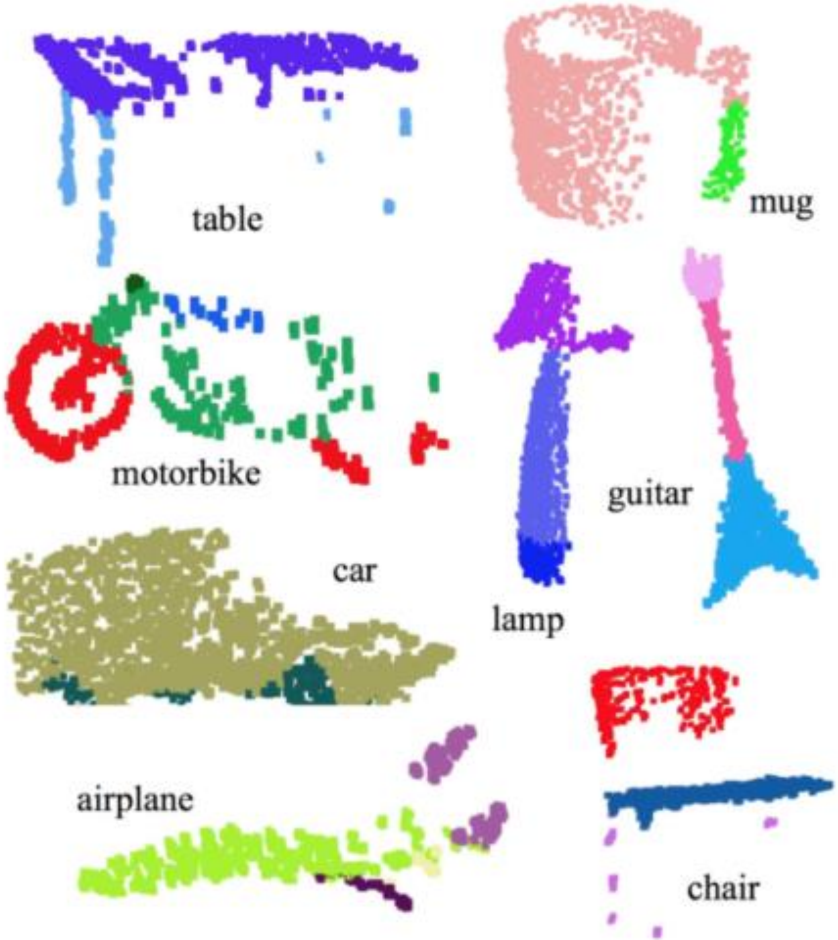
$$f(X) = \rho\left(\sum_{x \in X} \phi(x)\right) \longrightarrow f(X) = \rho\left(\sum_{x \in X} \alpha(w, x)\phi(x)\right)$$

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

Deep Sets

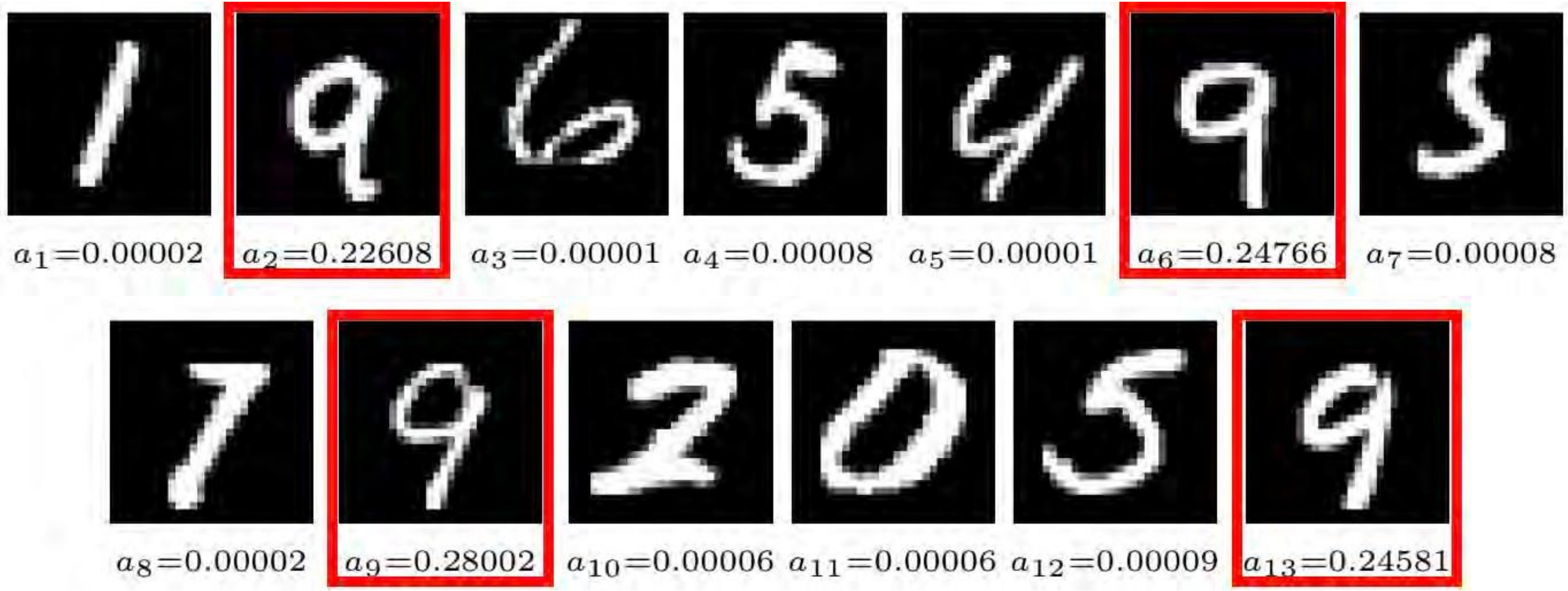


point clouds



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

Identifying sets that contain the digit ‘9’



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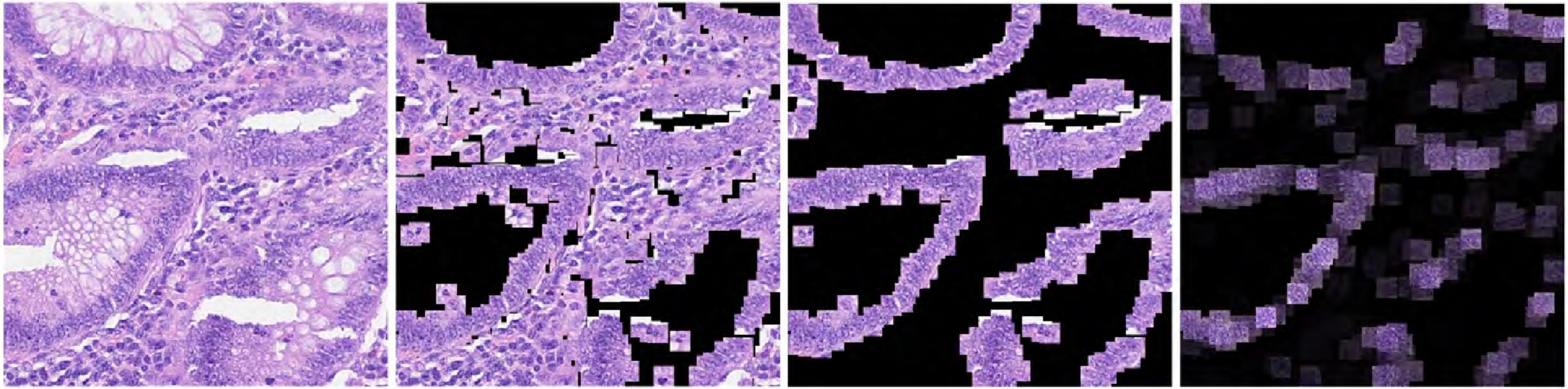


tissue sample

windowed cell nuclei

cancerous cells

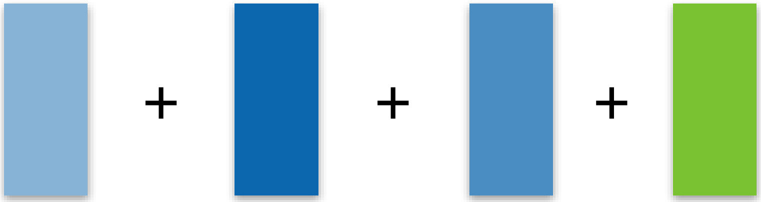
attention weights

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

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

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

The tutorial is awesome.



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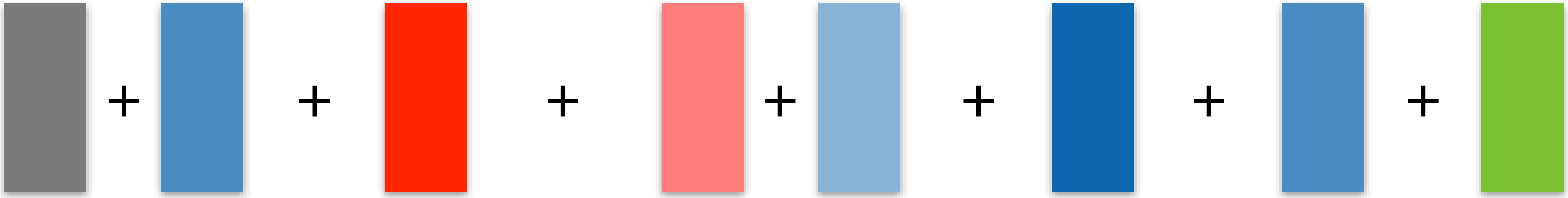
$$f(X) = \rho\left(\sum_{i=1}^{n} \phi(w_i)\right)$$

Alex is obnoxious but the tutorial is awesome.



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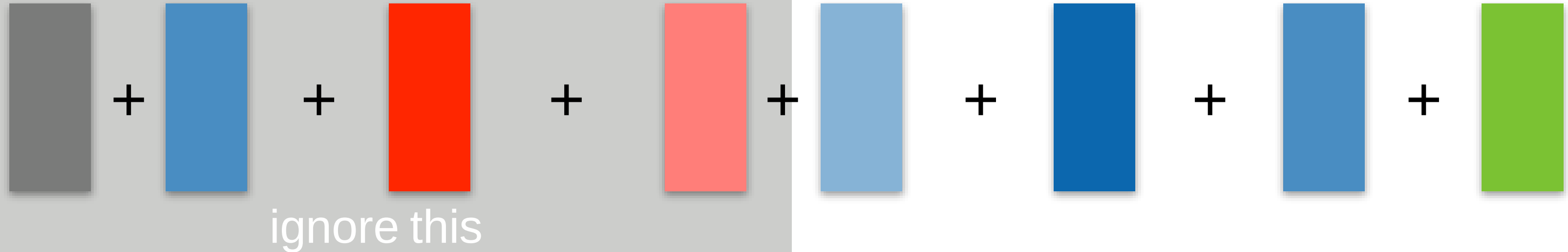
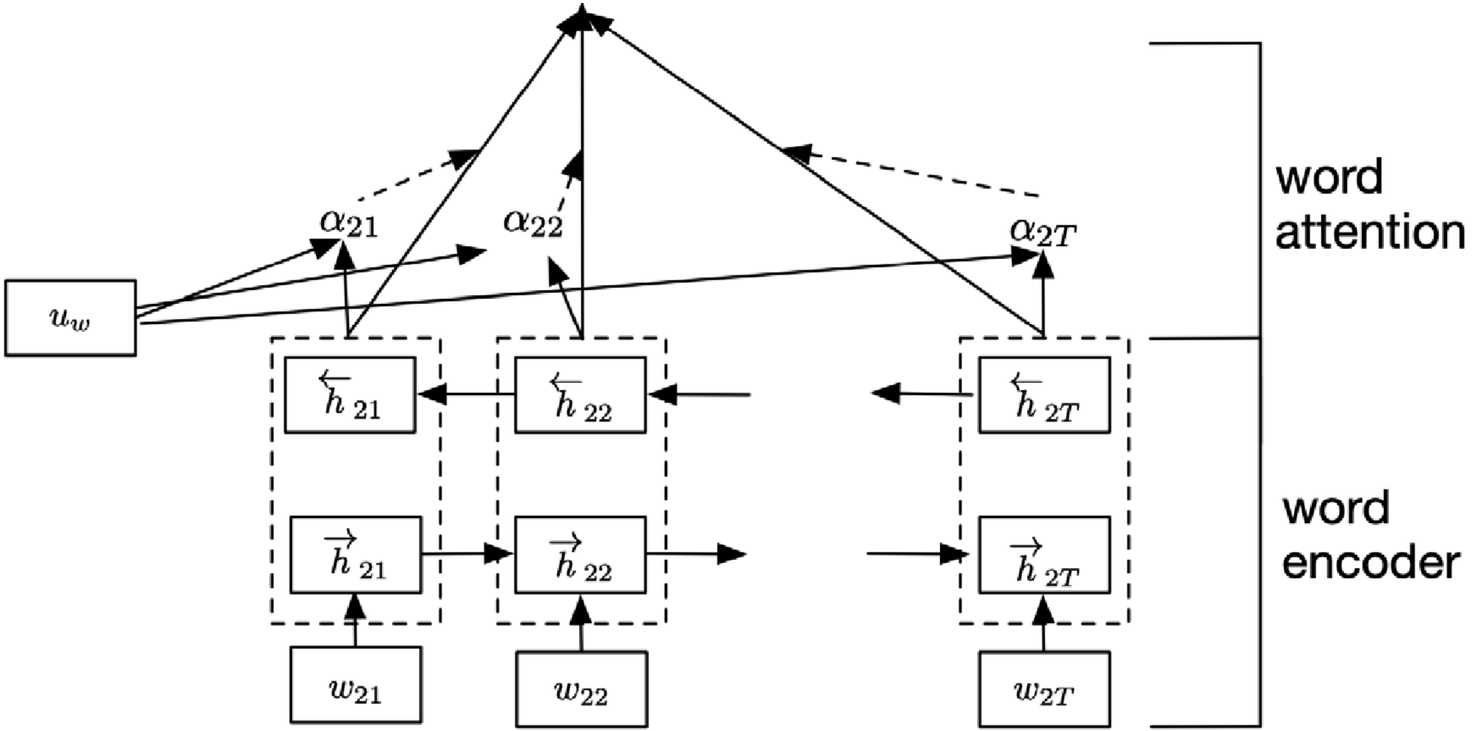


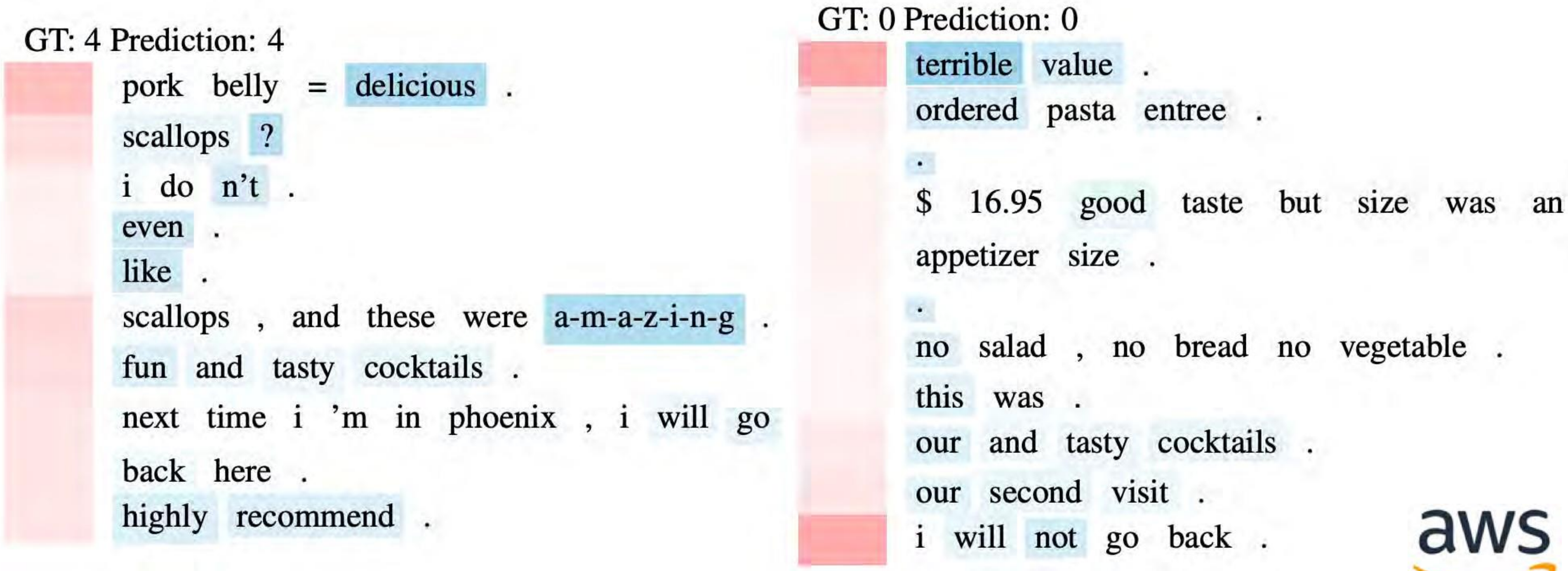
Attention weighting for documents (Wang et al, ’16)

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



Hierarchical attention weighting (Yang et al. ’17)

Some sentences are more important than others …



Hierarchical attention

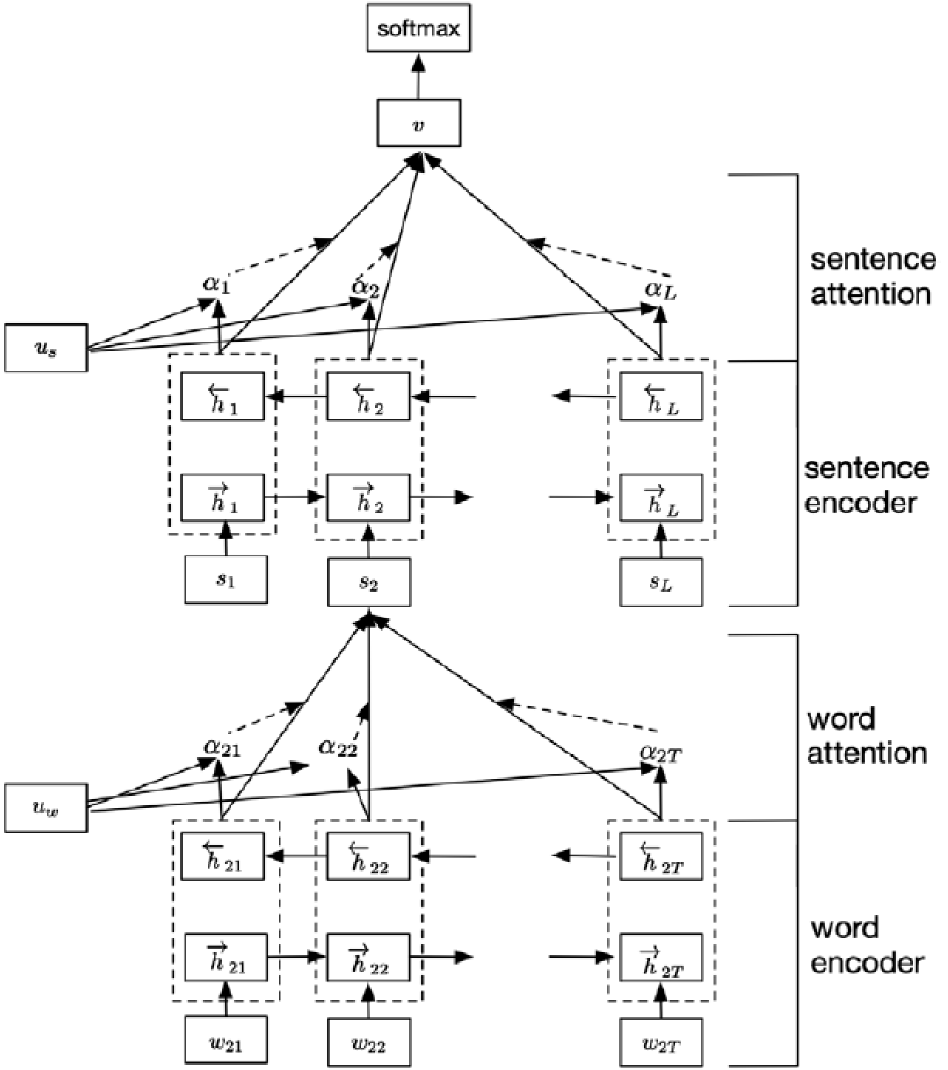
- Word level

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

- Sentence level

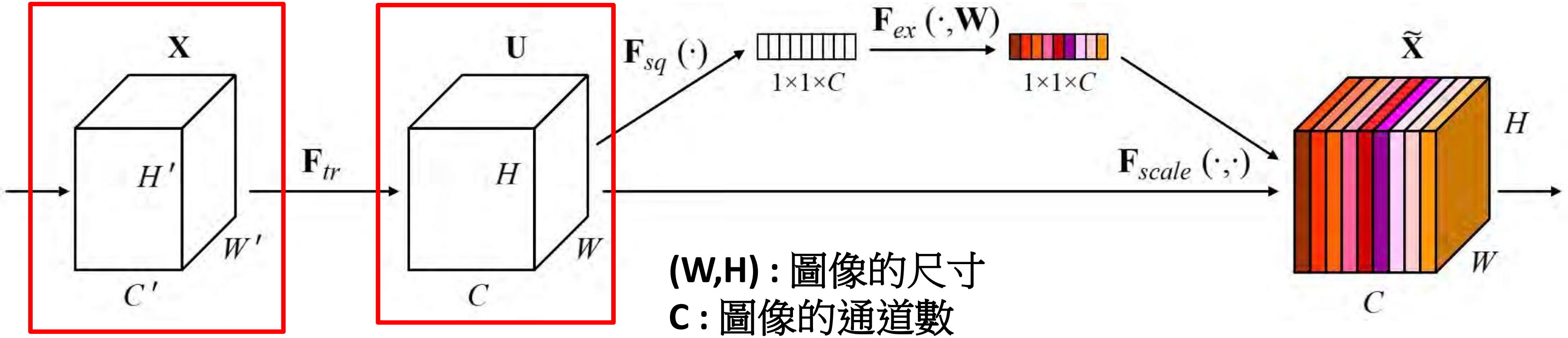
$$g(d) = \rho\left(\sum_{i=1}^{n} \alpha(s_i, d)\phi(f(s_i))\right)$$

- Embeddings e.g. via GRU



More Applications

Squeeze Excitation Networks (Hu et al., ’18)

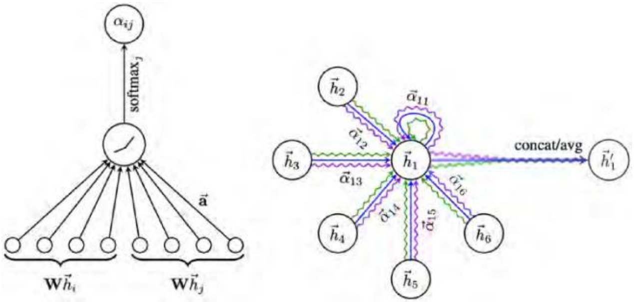


(W,H) : 圖像的尺寸
C : 圖像的通道數

Feature map

Graph Attention Networks

(Velickovic et al., ’18)



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

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